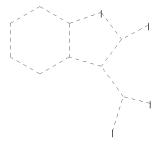
=>

Uploading C:\Program Files\Stnexp\Queries\10580610-registry-interm.str



chain nodes : 11 12 13 14 ring nodes : 1 2 3 4 5 6 7 8 9 chain bonds : 8-11 9-12 12-13 12-14 ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 exact/norm bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 8-11 \quad 9-12 \quad 12-13 \quad 12-14$ isolated ring systems :

containing 1 :

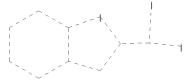
Match level:

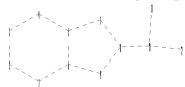
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L4STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10580610-registry-interm-2.str





chain nodes : 10 11 12 ring nodes : 1 2 3 4 5 6 7 8 9 chain bonds : 8-10 10-11 10-12 ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 8-10 \quad 10-11 \quad 10-12$

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS

```
L6
       STRUCTURE UPLOADED
                STRUCTURE UPLOADED
L4
             31 S L4
L5
                STRUCTURE UPLOADED
L6
             50 S L6
L7
L8
            501 S L4 SSS FULL
L9
          28071 S L6 SSS FULL
     FILE 'CAPLUS' ENTERED AT 08:55:17 ON 05 MAY 2008
           201 S L8
L10
           9784 S L9
L11
             31 S L10 AND L11
L12
L13
              2 S US200!-580610/APPS
L14
              1 S L12 AND L13
L15
             30 S L12 NOT L13
```

FILE 'REGISTRY' ENTERED AT 08:55:53 ON 05 MAY 2008

=> d 14

L4 HAS NO ANSWERS

L4 STR

Structure attributes must be viewed using STN Express query preparation.

=> d 16 L6 HAS NO ANSWERS L6 STR

Structure attributes must be viewed using STN Express query preparation.

L15 ANSWER 1 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:299076 CAPLUS <<LOGINID::20080505>>

DN 146:482222

TI Oxidative Rearrangement of Indoles: A New Approach to the EFHG-Tetracyclic Core of Diazonamide A

AU Poriel, Cyril; Lachia, Mathilde; Wilson, Claire; Davies, James R.; Moody, Christopher J.

CS Department of Chemistry, University of Exeter, Exeter, EX4 4QD, UK

SO Journal of Organic Chemistry (2007), 72(8), 2978-2987 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 146:482222

GΙ

AB A new approach to the ring EFHG-tetracyclic core fragment of the marine secondary metabolite diazonamide A is described. The route is based on the oxidative rearrangement of 3-arylindole-2-carboxylates. Thus, a range of 3-arylindole-2-carboxylates, for example I (X = H, Br; PMB = CH2C6H4OMe-4), underwent rearrangement to the corresponding 3,3-disubstituted oxindoles, for example II, with migration of the ester group upon treatment with tert-Bu hypochlorite followed by acid. II with a 3-[2-(4-methoxybenzyloxy)]phenyl substituent underwent cyclization to the tetracyclic aminals III (X = H, R = t-Bu; X = H, R = CH2CH:CH2; X = Br, R = CH2CH:CH2) following N-protection, reduction, and treatment with methanesulfonic anhydride. The methodol. was applied to tyrosine-indole derivative IV to give the EFHG-tetracyclic core of diazonamide A.

II 935846-44-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; preparation of tetracyclic ring EFHG core of diazonamide A using oxidative rearrangement of arylindolecarboxylates)

RN 935846-44-9 CAPLUS

CN 1H-Indole-1,3-dicarboxylic acid, 2,3-dihydro-3-[2-[(4-methoxyphenyl)methoxy]phenyl]-2-oxo-, 1-(1,1-dimethylethyl) 3-ethyl ester (CA INDEX NAME)

IT 3770-50-1 16732-69-7

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of tetracyclic ring EFHG core of diazonamide A using oxidative

rearrangement of arylindolecarboxylates)

RN 3770-50-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, ethyl ester (CA INDEX NAME)

RN 16732-69-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-bromo-, ethyl ester (CA INDEX NAME)

IT 117637-79-3P 935846-32-5P 935846-35-8P 935846-38-1P 935846-40-5P 935846-41-6P 935846-42-7P 935846-43-8P 935846-45-0P 935846-46-1P 935846-54-1P 935846-55-2P 935846-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetracyclic ring EFHG core of diazonamide A using oxidative rearrangement of arylindolecarboxylates)

RN 117637-79-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-iodo-, ethyl ester (CA INDEX NAME)

RN 935846-32-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-bromo-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 935846-35-8 CAPLUS

CN 1H-Indole-3-carboxylic acid, 7-bromo-2,3-dihydro-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 935846-38-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-bromo-3-iodo-, ethyl ester (CA INDEX NAME)

RN 935846-40-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[2-[(4-methoxyphenyl)methoxy]phenyl]-, ethyl ester (CA INDEX NAME)

RN 935846-41-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-bromo-3-[2-[(4-methoxyphenyl)methoxy]phenyl]-, ethyl ester (CA INDEX NAME)

RN 935846-42-7 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-[2-[(4-methoxyphenyl)methoxy]phenyl]-2-oxo-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & H & O \\ \hline & N & O \\ \hline & C - OEt \\ \hline & O \\ \hline \\ MeO \end{array}$$

RN 935846-43-8 CAPLUS

CN 1H-Indole-3-carboxylic acid, 7-bromo-2,3-dihydro-3-[2-[(4-methoxyphenyl)methoxy]phenyl]-2-oxo-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{Br} \\ \text{H} \\ \text{O} \\ \text{CH}_2 - \text{O} \\ \end{array}$$

RN 935846-45-0 CAPLUS

CN 1H-Indole-1,3-dicarboxylic acid, 2,3-dihydro-3-[2-[(4-methoxyphenyl)methoxy]phenyl]-2-oxo-, 3-ethyl 1-(2-propen-1-yl) ester (CA INDEX NAME)

$$\begin{array}{c|c} O \\ C - O - CH_2 - CH = CH_2 \\ \hline N & O \\ \hline C - OEt \\ O \\ \hline MeO \end{array}$$

RN 935846-46-1 CAPLUS

CN 1H-Indole-1,3-dicarboxylic acid, 7-bromo-2,3-dihydro-3-[2-[(4-methoxyphenyl)methoxy]phenyl]-2-oxo-, 3-ethyl 1-(2-propen-1-yl) ester (CA INDEX NAME)

Br
$$C-O-CH_2-CH=CH_2$$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$
 $C-O-CH_2-CH=CH_2$

RN 935846-54-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-bromo-3-[5-[(2S)-3-(1,1-dimethylethoxy)-3-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]-2-[(4-

methoxyphenyl)methoxy]phenyl]-, ethyl ester (CA INDEX NAME)
Absolute stereochemistry. Rotation (+).

PAGE 1-A

PAGE 2-A

RN 935846-55-2 CAPLUS

CN 1H-Indole-3-carboxylic acid, 7-bromo-3-[5-[(2S)-3-(1,1-dimethylethoxy)-3-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]-2-[(4-methoxyphenyl)methoxy]phenyl]-2,3-dihydro-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A || O

RN 935846-58-5 CAPLUS
CN 1H-Indole-1,3-dicarboxylic acid, 7-bromo-3-[5-[(2S)-3-(1,1-dimethylethoxy)-3-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]-2-[(4-methoxyphenyl)methoxy]phenyl]-2,3-dihydro-2-oxo-, 3-ethyl 1-(2-propen-1-yl) ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A

0

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L15 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2003:867664 CAPLUS <<LOGINID::20080505>>
- DN 140:93957
- TI Synthesis of benzothiopyrano[2,3-b]indol-11-one and benzopyrano[2,3-b]indol-11-one
- AU Engqvist, Robert; Bergman, Jan
- CS Karolinska Institute, Department of Biosciences at Novum, Unit for Organic Chemistry, CNT, Huddinge, SE-141 57, Swed.
- SO Tetrahedron (2003), 59(48), 9649-9653 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier Science B.V.
- DT Journal
- LA English
- OS CASREACT 140:93957
- AB The fused heterocycles benzothiopyrano[2,3-b]indol-11-one and benzopyrano[2,3-b]indol-11-one, have been prepared from Me 3-indolecarboxylate in two steps.
- IT 645388-39-2P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cyclization of; preparation of benzothiopyranoindolone and benzopyranoindolone derivs. from their corresponding

indolecarboxylates)

RN 645388-39-2 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2-phenoxy-, methyl ester (CA INDEX NAME)

IT 3770-50-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzothiopyranoindolone and benzopyranoindolone derivs. from their corresponding indolecarboxylates)

RN 3770-50-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, ethyl ester (CA INDEX NAME)

IT 106184-17-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzothiopyranoindolone and benzopyranoindolone derivs. from their corresponding indolecarboxylates)

RN 106184-17-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-(phenylthio)-, ethyl ester (CA INDEX NAME)

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2003:18743 CAPLUS <<LOGINID::20080505>>

DN 138:303806

 \mbox{TI} 3,3-sigmatropic rearrangements involving N-O bond-cleavage of enehydroxylamine derivatives

AU Reis, Lucinda V.; Lobo, Ana M.; Prabhakar, Sundaresan; Duarte, Mariana P.

CS Departamento de Quimica, CQFB/REQUIMTE, Faculdade de Ciencias e

Tecnologia, Universidade Nova de Lisboa, Monte da Caparica, 2829, Port.

SO European Journal of Organic Chemistry (2003), (1), 190-208 CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

OS CASREACT 138:303806

AB Enehydroxylamines, derived from carbocyclic and heterocyclic 1,3-dioxo compds., react with a variety of unsatd. electrophiles to give, in good to excellent yields, substances that in general undergo 3,3-sigmatropic rearrangements either spontaneously or upon heating. In those cases in which such reactions failed, addition of sodium hydride was found to induce the transformation. A study of the rearrangement by use of deuterium-labeled compds. showed that no crossover occurs, indicating the intramol. nature of the process. The method provides 2,3- or 3,4-disubstituted cyclohexenones, 5,6-disubstituted barbiturates and the corresponding fused pyrrole and imidazolinone derivs.

IT 142836-67-7P 156301-06-3P 156301-07-4P 510773-39-4P 510773-40-7P 510773-41-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(sigmatropic rearrangements involving nitrogen-oxygen bond-cleavage of enehydroxylamine derivs.)

RN 142836-67-7 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 4,5,6,7-tetrahydro-1,6,6-trimethyl-4-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

RN 156301-06-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3,4,5,6,7-hexahydro-2-hydroxy-1-methyl-4-oxo-, methyl ester (CA INDEX NAME)

RN 156301-07-4 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3,4,5,6,7-hexahydro-2-hydroxy-1,6,6-trimethyl-4-oxo-, methyl ester (CA INDEX NAME)

RN 510773-39-4 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 2,3,4,5,6,7-hexahydro-2-hydroxy-1-methyl-4-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

RN 510773-40-7 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 4,5,6,7-tetrahydro-1-methyl-4-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

RN 510773-41-8 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 2,3,4,5,6,7-hexahydro-2-hydroxy-1,6,6-trimethyl-4-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:861062 CAPLUS <<LOGINID::20080505>>

DN 139:197300

TI Product class 13: indole and its derivatives

AU Joule, J. A.

CS Department of Chemistry, University of Manchester, Manchester, M13 9PL, UK

SO Science of Synthesis (2001), 10, 361-652 CODEN: SSCYJ9

PB Georg Thieme Verlag

DT Journal; General Review

LA English

ΙT

AB A review of preparation of indoles and its derivs. Covered reactions include cyclization, ring transformation, aromatization and substituent modifications. Subclasses covered include 1H-indol-1-ols, 1,3-dihydro-2H-indol-2-ones, and 1,2-dihydro-3H-indol-3-ones.

4382-54-1 37493-34-8 53252-66-7

153827-71-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indoles and analogs thereof via cyclization, ring
transformation, aromatization and substituent modifications)

RN 4382-54-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-methoxy- (CA INDEX NAME)

RN 37493-34-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-methyl-, methyl ester (CA INDEX NAME)

RN 53252-66-7 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 4,5,6,7-tetrahydro-1-methyl-, dimethyl ester (9CI) (CA INDEX NAME)

RN 153827-71-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-iodo-1-(phenylsulfonyl)-, ethyl ester (CA INDEX NAME)

2400-35-3P 3770-50-1P 4966-40-9P ΙT 16381-42-3P 16732-64-2P 21139-32-2P 21183-59-5P 36004-74-7P 36800-67-6P 39478-72-3P 39731-09-4P 54781-93-0P 58664-93-0P 66552-21-4P 66552-23-6P 66552-39-4P 66552-40-7P 77069-10-4P 82633-34-9P 91559-45-4P 94527-32-9P 96277-44-0P 104681-05-2P 107517-71-5P 113525-31-8P 119581-01-0P 121045-66-7P 172216-95-4P 172516-96-0P 182180-07-0P 207739-39-7P 207739-53-5P 582319-01-5P 582319-19-5P 582319-34-4P 582319-49-1P 582319-50-4P 582320-02-3P 582320-15-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of indoles and analogs thereof via cyclization, ring transformation, aromatization and substituent modifications) RN 2400-35-3 CAPLUS CN 1H-Indole-2-carboxylic acid, 6-methoxy-3-methyl-, ethyl ester (CA INDEX NAME)

CN 1H-Indole-2-carboxylic acid, ethyl ester (CA INDEX NAME)

RN 4966-40-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5,6-bis(phenylmethoxy)- (CA INDEX NAME)

RN 16381-42-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-methoxy-3-methyl-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & O \\ & \parallel \\ N & C-OEt \end{array}$$

RN 16732-64-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-bromo- (CA INDEX NAME)

RN 21139-32-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 21183-59-5 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 1-cyclohexyl-5-hydroxy-, dimethyl ester (9CI) (CA INDEX NAME)

RN 36004-74-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(4-methylphenyl)sulfonyl]-3-phenyl-, methyl ester (CA INDEX NAME)

RN 36800-67-6 CAPLUS

CN 1H-Indole-2, 4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro- (CA INDEX NAME)

RN 39478-72-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-1-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 39731-09-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-(phenylmethoxy)- (CA INDEX NAME)

$$\begin{array}{c} \text{H} \\ \text{N} \\ \text{CO}_2\text{H} \\ \\ \text{Ph-CH}_2\text{-O} \end{array}$$

RN 54781-93-0 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 2,3-dimethyl ester (CA INDEX NAME)

RN 58664-93-0 CAPLUS

CN 1H-Indole-3-acetic acid, 2-carboxy-1-methyl- (CA INDEX NAME)

RN 66552-21-4 CAPLUS

CN 1H-Indole-2,6-dicarboxylic acid, 3-methyl-, 2-ethyl 6-methyl ester (CA INDEX NAME)

RN 66552-23-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-bromo-3-methyl-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} \text{Br} & \overset{\text{O}}{\parallel} \\ \text{N} & \text{C-OEt} \\ \\ \text{Me} \end{array}$$

RN 66552-39-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-3-methyl-, ethyl ester (CA INDEX NAME)

RN 66552-40-7 CAPLUS

CN 1H-Indole-2,5-dicarboxylic acid, 3-methyl-, 2-ethyl 5-methyl ester (CA INDEX NAME)

RN 77069-10-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-acetyl-, ethyl ester (CA INDEX NAME)

RN 82633-34-9 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 1-methyl-, dimethyl ester (9CI) (CA INDEX NAME)

RN 91559-45-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-methyl-5-nitro-, ethyl ester (CA INDEX NAME)

$$O_2N$$
 H
 C
 C
 OEt

RN 94527-32-9 CAPLUS

CN 5H-1,3-Dioxolo[4,5-f]indole-6-carboxylic acid, ethyl ester (CA INDEX NAME)

RN 96277-44-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 104681-05-2 CAPLUS

CN 1H-Benz[g]indole-2-carboxylic acid, 3-methyl-, methyl ester (CA INDEX NAME)

RN 107517-71-5 CAPLUS

CN 1H-Indole-2,4-dicarboxylic acid, diethyl ester (9CI) (CA INDEX NAME)

RN 113525-31-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-hydroxy-1-phenyl-5-(phenylmethoxy)-, methyl

ester (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{O} \\ & \parallel & \text{C-OMe} \\ \\ \text{Ph-CH}_2-\text{O} & \text{OH} \end{array}$$

RN 119581-01-0 CAPLUS

CN 1H-Indole-2,6,7-tricarboxylic acid, 1-methyl-, trimethyl ester (9CI) (CA INDEX NAME)

RN 121045-66-7 CAPLUS

CN 1H-Benz[f]indole-2-carboxylic acid, 9-methoxy-1-(phenylmethyl)-, ethyl ester (CA INDEX NAME)

RN 172216-95-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-phenyl-7-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)

RN 172516-96-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-amino-5-methoxy-6-methyl-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{H} & \text{C-OMe} \\ \hline \text{MeO} & \text{NH}_2 \\ \end{array}$$

RN 182180-07-0 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinoline-2-carboxylic acid, 4-(2,2-dimethyl-1-oxopropoxy)-, methyl ester (CA INDEX NAME)

RN 207739-39-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-(acetylamino)-7-(2-hydroxyethoxy)-4-propyl-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & \text{N-Pr} & \text{O} \\ & \text{C-OMe} \\ & \text{NH} \\ & \text{HO-CH}_2\text{-CH}_2\text{-O} \end{array}$$

RN 207739-53-5 CAPLUS

CN 1H-Indole-2,5-dicarboxylic acid, 7-(2-hydroxyethoxy)-4-methyl-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \text{Me} & O \\ \parallel & \parallel & C \\ \hline \text{MeO-C} & & \text{NH} \\ \\ \text{HO-CH}_2\text{-CH}_2\text{-O} & & \\ \end{array}$$

RN 582319-01-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[2-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

RN 582319-19-5 CAPLUS

CN Benz[cd]indole-2-carboxylic acid, 1,3,4,5-tetrahydro- (CA INDEX NAME)

RN 582319-34-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-bromo-3-methyl-7-(phenylmethoxy)-1-(phenylsulfonyl)-, ethyl ester (CA INDEX NAME)

RN 582319-49-1 CAPLUS

CN 1H-Indole-2,7-dicarboxylic acid, 3-methyl-, 2-ethyl 7-methyl ester (CA INDEX NAME)

RN 582319-50-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-methyl-6-(phenylmethyl)-, ethyl ester (CA INDEX NAME)

RN 582320-02-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-(phenylsulfonyl)-3-(2-thiazolyl)-, ethyl ester (CA INDEX NAME)

RN 582320-15-8 CAPLUS

CN 1H-Indole-3-carboxylic acid, 1-ethyl-2,3-dihydro-2-oxo-, ethyl ester (CA INDEX NAME)

RE.CNT 1348 THERE ARE 1348 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2001:896214 CAPLUS <<LOGINID::20080505>>

DN 136:241026

 ${\tt TI}$ The potential of 19F NMR spectroscopy for rapid screening of cell cultures for models of mammalian drug metabolism

AU Corcoran, Olivia; Lindon, John C.; Hall, Richard; Ismail, Ismail M.; Nicholson, Jeremy K.

CS Biological Chemistry, Division of Biomedical Sciences, Imperial College of Science, Technology and Medicine, London, SW7 2AZ, UK

SO Analyst (Cambridge, United Kingdom) (2001), 126(12), 2103-2106 CODEN: ANALAO; ISSN: 0003-2654

PB Royal Society of Chemistry

DT Journal

LA English

AΒ The use of microbial cultures as a complementary model for mammalian drug metabolism has been well established previously. Here is a preliminary investigation into the potential of 19F NMR spectroscopy as a rapid screening tool to quantify the biotransformations of fluorine-containing model drugs. Biotransformations of three model drugs in 48 taxonomically diverse organisms were measured by acquiring 19F NMR spectra at 376 MHz. The presence of fluorine in the mols. allowed rapid, simultaneous detection of over 20 biotransformation products without sample pre-treatment, chromatog., mass spectrometric techniques or the use of radiolabeled substrates. The detection limit at 376 MHz using 5 mm NMR tubes was 0.3 μg ml-1 using a typical anal. time of 20 min per sample. With the recent advent of flow injection NMR technol., anal. time of 5 min could be achieved with less sample. This approach may be used to develop fast small-scale microbial screens for the biosynthesis of metabolite stds. and production of novel drug analogs, while also having a role in reducing animal expts. needed to identify animal and human metabolites of fluorinated xenobiotics.

RL: PKT (Pharmacokinetics); BIOL (Biological study)

(potential of 19F NMR spectroscopy for rapid screening of cell cultures for models of mammalian drug metabolism)

RN 399-76-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-fluoro- (CA INDEX NAME)

RN 144625-67-2 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5-fluoro-2-methoxy-, [1-[2- [(methylsulfonyl)amino]ethyl]-4-piperidinyl]methyl ester (CA INDEX NAME)

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1998:49527 CAPLUS <<LOGINID::20080505>>

DN 128:167288

TI Synthesis of nitrogen and sulfur analogs of the seco-CI alkylating agent

AU Tercel, Moana; Denny, William A.

CS Faculty of Medicine and Health Science, Cancer Research Laboratory, The University of Auckland, Auckland, N. Z.

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (3), 509-520 CODEN: JCPRB4; ISSN: 0300-922X

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 128:167288

GΙ

AB Two complementary syntheses of amino seco-CI (CI = 1a,2,3,5-tetrahydro-1H-cycloprop[1,2-c]indol-5-one) alkylating agents, e.g. I (R1 = 03SMe, R2 = S02Me; R1 = Cl, R2 = H) and II, starting from isomeric chloronitrobenzoic acids are reported. Further reactions of these compds., including diazotization to phenol and thiophenol derivs., and alkylation and acylation reactions relevant to the preparation of pro-drug forms are also described.

IT 128781-07-7

RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of nitrogen and sulfur analogs of seco-CI alkylating agent)

RN 128781-07-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5,6,7-trimethoxy- (CA INDEX NAME)

IT 185433-47-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of nitrogen and sulfur analogs of seco-CI alkylating agent)

RN 185433-47-0 CAPLUS

CN 3H-Indole-3,3-dicarboxylic acid, 1,2-dihydro-6-nitro-2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O_2N & & H & O & O \\ \hline & N & & O & C \\ \hline & C-OMe & \\ & O & \\ \end{array}$$

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1998:14365 CAPLUS <<LOGINID::20080505>>

DN 128:114847

TI Palladium-catalyzed reactions of indolic triflate with allylic alcohols

AU Malapel-Andrieu, Beatrice; Merour, Jean-Yves

CS Inst. Chim. Org. Anal., Univ. Orleans, Orleans, 45067, Fr.

SO Tetrahedron Letters (1998), 39(1/2), 39-42 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 128:114847

GΙ

AB Reactions of 3-indolic triflate I with allylic alcs. RCH:CH(CH2)mCHR'OH(R, R' = H, Me, m = 0, 1) in presence of palladium (II) acetate gave access to aldehydic compds., e.g., II, and in a more surprising way to C-2 substituted products and oxoindole derivs., e.g., III.

IT 31827-04-0 42871-90-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(palladium-catalyzed addition of indolic triflate to allylic alcs.)

RN 31827-04-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-hydroxy-, methyl ester (CA INDEX NAME)

RN 42871-90-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-hydroxy-1-methyl-, ethyl ester (CA INDEX NAME)

IT 201665-48-7P 201665-54-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(palladium-catalyzed addition of indolic triflate to allylic alcs.)

RN 201665-48-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-methyl-3-[[(trifluoromethyl)sulfonyl]oxy]-, ethyl ester (CA INDEX NAME)

RN 201665-54-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-1-methyl-3-oxo-2-(3-oxopropyl)-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & \text{C}-\text{OEt} \\ \text{N} & \text{CH}_2-\text{CH}_2-\text{CHO} \\ \\ \text{O} & \\ \end{array}$$

IT 201665-47-6P 201665-49-8P 201665-50-1P

201665-51-2P 201665-52-3P 201665-53-4P

201665-55-6P 201665-56-7P 201665-57-8P RL: SPN (Synthetic preparation); PREP (Preparation)

(palladium-catalyzed addition of indolic triflate to allylic alcs.)

RN 201665-47-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[[(trifluoromethyl)sulfonyl]oxy]-, methyl ester (CA INDEX NAME)

RN 201665-49-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-1-methyl-3-oxo-2-(2-propenyloxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 201665-50-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2-(2-butenyloxy)-2,3-dihydro-1-methyl-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & \text{II} \\ \text{N} & \text{C-OEt} \\ \text{O-CH}_2\text{-CH} \\ \text{CH-Me} \\ \\ \text{O} \end{array}$$

RN 201665-51-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2-(3-butenyloxy)-2,3-dihydro-1-methyl-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 201665-52-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-hydroxy-1-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 201665-53-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-methyl-3-(3-oxopropyl)-, ethyl ester (CA INDEX NAME)

RN 201665-55-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2-(diethylamino)-2,3-dihydro-1-methyl-3-oxo-, ethyl ester (CA INDEX NAME)

RN 201665-56-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2-(dimethylamino)-2,3-dihydro-1-methyl-3-oxo-, ethyl ester (CA INDEX NAME)

RN 201665-57-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-2-(3-hydroxypropyl)-1-methyl-3-oxo-, ethyl ester (CA INDEX NAME)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN AN 1997:257472 CAPLUS <<LOGINID::20080505>>

```
DN 126:238304
```

TI Preparation of seco precursors of cyclopropylindoles as anticancer drugs

IN Denny, William Alexander; Tercel, Moana

PA Auckland Division Cancer Society of New Zealand Inc., N. Z.; Denny, William Alexander; Tercel, Moana

SO PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

FAN.	PATENT NO.					KIND		DATE		APPLICATION NO.						DATE		
ΡI	WO 9	WO 9707097			A1 19970227			0227	WO 1996-NZ83					19960819				
	1	W: .	AL,	AM,	ΑT,	ΑU,	AZ,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,	DK,
			EE,	ES,	FI,	GB,	GE,	HU,	IL,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LK,	LR,
			LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,
			SD,	SE,	SG,	SI,	SK,	ΤJ,	TM,	TR,	ΤT,	UA,	UG,	US,	UZ,	VN		
		RW:	KΕ,	LS,	MW,	SD,	SZ,	UG,	ΑT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,
			ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM			
	CA 2229264				A1		1997	0227	CA 1996-2229264						19960819			
	AU 9667109			Α		1997	0312	AU 1996-67109						19960819				
	AU 707644			В2	19990715													
	EP 8	IP 850220				A1	19980701			EP 1996-927217					19960819			
		R: .	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LΙ,	LU,	NL,	SE,	MC,	PT,
	IE, FI																	
	JP 11511113					Τ	19990928			JP 1996-531337						19960819		
	US 5985909					Α		19991116			US 1998-11883					19980218		
PRAI	GB 1995-16943					Α		1995	0818									
	WO 1996-NZ83					W		1996	0819									
OS GI	MARP	MARPAT 126:238304																

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The title compds. [I and II; X = halo, OSO2R (wherein R = H, (un)substituted by 1-4 OH groups lower alkyl, (un)substituted by 1-2 lower alkyl groups NH2); Y = NH2, NO2, NHOH, etc.; E = N, CH; G = O, S, NH; Q = H, OR, NR2, etc.; R1 = R; P = III, IV, V (wherein Z = H, Me; n = 1-2; R2 = R, CONHR, NHCOR, OR, SO2R)], useful as prodrugs for antibody-directed enzyme-prodrug therapy (ADEPT) and gene-directed enzyme-prodrug therapy (GDEPT) for cancer, were prepared Thus, two alternative 10-step syntheses of VI, which showed IC50 of 0.32 μ M in AA8 cells, and against UV4 cells of 0.059 μ M, were described.

IT 128781-07-7

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of seco precursors of cyclopropylindoles as anticancer drugs)

RN 128781-07-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5,6,7-trimethoxy- (CA INDEX NAME)

IT 185433-47-0P 188538-12-7P 188538-13-8P

188538-14-9P 188538-15-0P 188538-16-1P

188538-17-2P 188538-18-3P 188538-19-4P

188538-20-7P 188538-21-8P 188538-22-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of seco precursors of cyclopropylindoles as anticancer drugs)

RN 185433-47-0 CAPLUS

CN 3H-Indole-3,3-dicarboxylic acid, 1,2-dihydro-6-nitro-2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O_2N & & H & O \\ & N & & O \\ & & C-\text{OMe} \\ & & O \\ & & O \\ \end{array}$$

RN 188538-12-7 CAPLUS

CN 1H-Indole-2,6-dicarboxylic acid, 6-(1,1-dimethylethyl) 2-methyl ester (CA INDEX NAME)

RN 188538-13-8 CAPLUS

CN 1H-Indole-2,6-dicarboxylic acid, 2-methyl ester (CA INDEX NAME)

RN 188538-14-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-(2-pyridinyl)ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

RN 188538-15-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-(2-pyridinyl)ethyl]amino]carbonyl]-(CA INDEX NAME)

RN 188538-16-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]-,
 methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ &$$

RN 188538-17-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]-(CA INDEX NAME)

RN 188538-18-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

RN 188538-19-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-hydroxy-1-(hydroxymethyl)amino]carbonyl]-, methyl ester (CA INDEX NAME)

RN 188538-20-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]carbonyl]- (CA INDEX NAME)

RN 188538-21-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

RN 188538-22-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-[[[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]carbonyl]- (CA INDEX NAME)

- L15 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 1996:197541 CAPLUS <<LOGINID::20080505>>
- DN 124:343046
- TI Synthesis of biindolyls by the reaction of indoles with indolin-2-ones and phosphoryl chloride or trifluoromethanesulfonic anhydride
- AU Black, David StC.; Ivory, Andrew J.; Kumar, Naresh
- CS School Chemistry, The Univ. New South Wales, Sydney, 2052, Australia
- SO Tetrahedron (1996), 52(13), 4697-708 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier
- DT Journal
- LA English
- OS CASREACT 124:343046
- AB Examples of 2,2'-, 2,3'-, and 2,7'-biindolyls have been prepared by the reaction of indoles with indolin-2-ones and phosphoryl chloride or trifluoromethanesulfonic anhydride. In certain conditions terindolyls can also be formed and those described contain combinations of the above linkages.
- IT 23659-85-0
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 (elimination reaction of)
- RN 23659-85-0 CAPLUS
- CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-hydroxy-4,6-dimethoxy-2-oxo-, ethyl ester (CA INDEX NAME)

- IT 105776-30-5
 - RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of biindolyls by the reaction of indoles with indolin-2-ones and phosphoryl chloride or trifluoromethanesulfonic anhydride)
- RN 105776-30-5 CAPLUS
- CN 1H-Indole-2,3-dicarboxylic acid, 4,6-dimethoxy-, dimethyl ester (9CI) (CA INDEX NAME)

IT 176722-78-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of biindolyls by the reaction of indoles with indolin-2-ones and phosphoryl chloride or trifluoromethanesulfonic anhydride)

RN 176722-78-4 CAPLUS

CN [2,7'-Bi-1H-indole]-2',3'-dicarboxylic acid, 4',6'-dimethoxy-, dimethyl ester (9CI) (CA INDEX NAME)

L15 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1996:193783 CAPLUS <<LOGINID::20080505>>

DN 124:343155

TI Antitumor heterocycles. Part 12. The synthesis of new hydroxypyrrolocarbazoles and hydroxypyridocarbazoles

AU Dharmasena, Priyanthi; Oliveira-Campos, Ana-M. F.; Querioz, Maria-Joao R. P.; Shannon, Patrick V. R.

CS School of Chemistry, Univ. of Wales, Cardiff, CF1 3TB, UK

SO Journal of Chemical Research, Synopses (1996), (1), 12-13 CODEN: JRPSDC; ISSN: 0308-2342

PB Royal Society of Chemistry

DT Journal

LA English

AB 7-Methoxy-8-pivaloyloxy-5,11-dimethyl- and 8-hydroxy-7-methoxy-5,11-dimethyl-pyrido[4,3-b] carbazoles have been synthesized from 6-hydroxy-7-methoxyindole and 6-acetoxy-7-methoxyindole; alternative routes from the indoles give the [2,3-f] and [3,2-f] isomers of hydroxymethoxypyrrolocarbazoles and acetoxymethoxypyrrolocarbazoles.

IT 157578-59-1P 176720-15-3P 176720-20-0P

176720-24-4P

RN 157578-59-1 CAPLUS

CN Pyrrolo[3,2-b]carbazole-2-carboxylic acid, 7-(acetyloxy)-1,5-dihydro-6-methoxy-3,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 176720-15-3 CAPLUS

CN Pyrrolo[3,2-b]carbazole-2-carboxylic acid, 1,5-dihydro-7-hydroxy-6-methoxy- 3,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 176720-20-0 CAPLUS

CN 1H-Indole-3-carboxylic acid, 3-[(2,3-dimethoxyphenyl)amino]-2,3-dihydro-6,7-dimethoxy-2-oxo-, ethyl ester (CA INDEX NAME)

RN 176720-24-4 CAPLUS

CN Pyrrolo[2,3-b]carbazole-2-carboxylic acid, 7-(acetyloxy)-1,9-dihydro-8-methoxy-3,4-dimethyl-, ethyl ester (CA INDEX NAME)

IT 176720-21-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of new hydroxypyrrolocarbazoles and hydroxypyridocarbazoles) $176720 - 21 - 1 \quad \text{CAPLUS}$

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-hydroxy-6,7-dimethoxy-2-oxo-, ethyl ester (CA INDEX NAME)

L15 ANSWER 11 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1994:482949 CAPLUS <<LOGINID::20080505>>

DN 121:82949

TI Reaction of ethyl acylindole-2-carboxylates with thallium trinitrate. Synthetic studies on indoles and related compounds. XXXIII

AU Tani, Masanobu; Matsumoto, Shigenobu; Aida, Yoshiyuki; Arikawa, Shiho; Nakane, Atsuko; Yokoyama, Yuusaku; Murakami, Yasuoki

CS Sch. Pharm. Sci., Toho Univ., Funabashi, 274, Japan

SO Chemical & Pharmaceutical Bulletin (1994), 42(3), 443-53 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

OS CASREACT 121:82949

GΙ

RN

AB Et acylindole-2-carboxylates (I; R = COMe, COEt, R1 = H, Me; R = H, R1 = COMe, COEt), were treated with thallium trinitrate (TTN) in methanol, Me orthoformate, Me orthoformate/sulfuric acid, and acetic acid. The reactions in the former three methanolic solvents gave Me indoleacetate derivs., e.g. [I; R = CH2CO2Me, CHMeCO2Me, CH(OMe)CO2Me, CMe(OMe)CO2Me, R1 = H, Me] via the Favorskii-type rearrangement reaction at the acyl group, whereas the reaction in acetic acid gave an oxindole derivative with rearrangement of the C2-ethoxycarbonyl group. This TTN reaction was applied to a model compound leading to the synthesis of lysergic acid. IT 31380-56-0 77069-10-4 92248-55-0

IT 31380-56-0 77069-10-4 92248-55-0 156361-86-3 156361-87-4 156361-88-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(Favorskii rearrangement/methoxylation of, with thallium trinitrate in methanolic solvents)

RN 31380-56-0 CAPLUS

RN 77069-10-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-acetyl-, ethyl ester (CA INDEX NAME)

RN 92248-55-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-acetyl-3-methyl-, ethyl ester (CA INDEX NAME)

RN 156361-86-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-(1-oxopropyl)-, ethyl ester (CA INDEX NAME)

RN 156361-87-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-(1-oxopropyl)-, ethyl ester (CA INDEX NAME)

RN 156361-88-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-methyl-5-(1-oxopropyl)-, ethyl ester (CA INDEX NAME)

IT 3770-50-1

RL: RCT (Reactant); RACT (Reactant or reagent) (acylation of, by aspartic acid chloride)

RN 3770-50-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, ethyl ester (CA INDEX NAME)

IT 90395-39-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (nitration of, with thallium trinitrate)

RN 90395-39-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-acetyl-, ethyl ester (CA INDEX NAME)

IT 26304-51-8
 RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation/rearrangement of, with thallium trinitrate)

RN 26304-51-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-methyl-, ethyl ester (CA INDEX NAME)

IT 42137-35-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and Favorskii rearrangement/methoxylation of, with thallium trinitrate)

RN 42137-35-9 CAPLUS

CN 1H-Cyclohept[cd]indole-2-carboxylic acid, 3,4,5,6-tetrahydro-6-oxo-, ethyl ester (CA INDEX NAME)

IT 156361-90-9P 156361-92-1P 156362-15-1P

156362-21-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acid hydrolysis of)

RN 156361-90-9 CAPLUS

CN 1H-Indole-3-acetic acid, 2-(ethoxycarbonyl)- α -methyl-, methyl ester (CA INDEX NAME)

RN 156361-92-1 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)- α -methyl-, methyl ester (CA INDEX NAME)

RN 156362-15-1 CAPLUS

CN 1H-Indole-3-butanoic acid, 2-(ethoxycarbonyl)-, methyl ester (CA INDEX NAME)

RN 156362-21-9 CAPLUS

CN 1H-Indole-3-butanoic acid, 2-(ethoxycarbonyl)- α [(trifluoroacetyl)amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 42137-33-7P 156362-22-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of)

RN 42137-33-7 CAPLUS

CN 1H-Indole-3-butanoic acid, 2-(ethoxycarbonyl)- (CA INDEX NAME)

RN 156362-22-0 CAPLUS

CN 1H-Indole-3-butanoic acid, 2-(ethoxycarbonyl)- α [(trifluoroacetyl)amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 156362-07-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and decarboxylation of)

RN 156362-07-1 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5-acetyl-2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

IT 156362-23-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and methoxylation of, with thallium trinitrate)

RN 156362-23-1 CAPLUS

CN 1H-Cyclohept[cd]indole-2-carboxylic acid, 3,4,5,6-tetrahydro-6-oxo-5-[(trifluoroacetyl)amino]-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 156362-20-8P

ΙT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

14750-19-7P 66552-40-7P 156361-89-6P

RN 156362-20-8 CAPLUS

CN 1H-Indole-3-butanoic acid, 2-(ethoxycarbonyl)- γ -oxo- α -

[(trifluoroacetyl)amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 66552-40-7 CAPLUS

CN 1H-Indole-2,5-dicarboxylic acid, 3-methyl-, 2-ethyl 5-methyl ester (CA INDEX NAME)

RN 156361-89-6 CAPLUS

CN 1H-Indole-3-acetic acid, 2-(ethoxycarbonyl)-, methyl ester (CA INDEX NAME)

RN 156361-91-0 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)-, methyl ester (CA INDEX NAME)

RN 156361-93-2 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)-3-methyl-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO-C-CH}_2 \\ \text{Me} \end{array}$$

RN 156361-94-3 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)- α ,3-dimethyl-, methyl ester (CA INDEX NAME)

RN 156361-95-4 CAPLUS

CN 1H-Indole-3-acetic acid, 2-(ethoxycarbonyl)- α -methoxy-, methyl ester (CA INDEX NAME)

RN 156361-96-5 CAPLUS

CN 1H-Indole-3-acetic acid, 2-(ethoxycarbonyl)- α -methoxy- α -methyl-, methyl ester (CA INDEX NAME)

RN 156361-97-6 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)- α -methoxy-, methyl ester (CA INDEX NAME)

RN 156361-98-7 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)- α -methoxy-3-methyl-, methyl ester (CA INDEX NAME)

RN 156361-99-8 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)- α -methoxy- α ,3-dimethyl-, methyl ester (CA INDEX NAME)

RN 156362-00-4 CAPLUS

CN 1H-Indole-3-acetic acid, 2-(methoxycarbonyl)-, methyl ester (CA INDEX NAME)

RN 156362-01-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-(2-methoxy-1-oxopropyl)-, methyl ester (CA INDEX NAME)

RN 156362-02-6 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)-3-methyl- α -oxo-, methyl ester (CA INDEX NAME)

RN 156362-03-7 CAPLUS

CN 1H-Indole-5-acetic acid, α -(dimethoxymethyl)-2-(ethoxycarbonyl)-3-methyl-, methyl ester (CA INDEX NAME)

RN 156362-04-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-(2-methoxy-1-oxopropyl)-3-methyl-, ethyl ester (CA INDEX NAME)

RN 156362-06-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-[(acetyloxy)acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 156362-09-3 CAPLUS

CN 1H-Indole-3-acetic acid, 2-(ethoxycarbonyl)- α -methyl- (CA INDEX NAME)

RN 156362-10-6 CAPLUS

CN 1H-Indole-5-acetic acid, 2-(ethoxycarbonyl)- α -methyl- (CA INDEX NAME)

RN 156362-11-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-acetyl-3-nitro-, ethyl ester (CA INDEX NAME)

RN 156362-12-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-acetyl-3-nitro-, ethyl ester (CA INDEX

NAME)

RN 156362-13-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-acetyl-, methyl ester (CA INDEX NAME)

RN 156362-16-2 CAPLUS

CN Benz[cd]indole-2,5-dicarboxylic acid, 1,3,4,5-tetrahydro-, 2-ethyl 5-methyl ester (CA INDEX NAME)

RN 156362-19-5 CAPLUS

CN 1H-Indole-5-butanoic acid, 2-(ethoxycarbonyl)- γ -oxo- α - [(trifluoroacetyl)amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 156362-24-2 CAPLUS

CN 1H-Cyclohept[cd]indole-2-carboxylic acid, 3,4,5,6-tetrahydro-3-methoxy-6-oxo-5-[(trifluoroacetyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

IT 133738-59-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction of)

RN 133738-59-7 CAPLUS

CN 1H-Indole-3-butanoic acid, 2-(ethoxycarbonyl)- γ -oxo-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & O \\ & | \\ & | \\ & C-OEt \\ & | \\ & C-CH_2-CH_2-C-OMe \\ & | \\ & | \\ & O \end{array}$$

L15 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1990:611747 CAPLUS <<LOGINID::20080505>>

DN 113:211747

OREF 113:35775a,35778a

TI The synthesis and chemistry of azolenines. Part 18. Preparation of 3-ethoxycarbonyl-3H-pyrroles via the Paal-Knorr reaction, and sigmatropic

rearrangements involving competitive ester migrations to C-2, C-4 and N $\,$

- AU Chiu, Pak Kan; Sammes, Michael P.
- CS Dep. Chem., Univ. Hong Kong, Hong Kong
- SO Tetrahedron (1990), 46(10), 3439-56 CODEN: TETRAB; ISSN: 0040-4020
- DT Journal
- LA English
- OS CASREACT 113:211747

GΙ

AB 3H-Pyrrole-3-carboxylic esters I [R1 = Me, Ph, CMe, CO2Et; R2 = Me, R3 = H, Me; R4 = Me, Ph, CMe3; R1R2 = (CH2)4, R3 = H, R4 = Me, Ph] were prepared, in some cases together with isomers having exocyclic double bonds, by cyclization. of suitably substituted 2-ethoxycarbonyl-1,4-diketones with liquid ammonia, followed by dehydration of the isolable 2-hydroxy-3,4-dihydro-2H-pyrrole intermediates with aluminia in boiling solvents. Prolonged heating in toluene or p-xylene converts the 3H-pyrroles (I) quant. into isomeric 4-esters II and N-esters III of 1H-pyrroles via competitive [1,5]sigmatropic rearrangements. Isolable intermediate 2H-pyrrole-2-carboxylic esters are converted similarly into the same products, under the same conditions. Detection of 3H-pyrroles as intermediates in the latter reaction demonstrates for the first time the reversibility of the thermal 2H-pyrrole to 3H-pyrrole interconversion.

IT 130460-17-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and dehydration of)

- RN 130460-17-2 CAPLUS
- CN 2H-Indole-3-carboxylic acid, 3,3a,4,5,6,7-hexahydro-2-hydroxy-2,3-dimethyl-, ethyl ester (CA INDEX NAME)

IT 130460-62-7P

- RN 130460-62-7 CAPLUS
- CN 2H-Indole-2-carboxylic acid, 4,5,6,7-tetrahydro-2,3-dimethyl-, ethyl ester (CA INDEX NAME)

L15 ANSWER 13 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1990:216513 CAPLUS <<LOGINID::20080505>>

DN 112:216513

OREF 112:36537a,36540a

TI Access to the three subunits of the antitumor antibiotic CC-1065 by hetero-Cope rearrangement of vinyl N-phenylhydroxamates

AU Martin, Pierre

CS Zent. Forschungslab., Ciba-Geigy A.-G., Basel, CH-4002, Switz.

SO Helvetica Chimica Acta (1989), 72(7), 1554-82 CODEN: HCACAV; ISSN: 0018-019X

DT Journal

LA German

OS CASREACT 112:216513

GΙ

AB The hetero-Cope rearrangement of vinyl N-phenylhydroxamates to indoles was used for the preparation of the 1,2-dihydro-3H,6H-benzo[1,2-b:4,3-b']dipyrrole skeleton I (R = Ac, R1 = H; R = SO2Ph, R1 = CH2Ph) the structural subunits characteristic of the antitumor antibiotic CC-1065 as well as the phosphodiesterase inhibitors PDE-I and PDE-II.

IT 127027-75-2P 127028-08-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acetylation of)

Ι

RN 127027-75-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-7-methoxy-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

RN 127028-08-4 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 3,6,7,8-tetrahydro-5-hydroxy-4-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

IT 127027-66-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and benzylation of)

RN 127027-66-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-hydroxy-7-methoxy-, ethyl ester (CA INDEX NAME)

IT 127027-65-0P 127028-09-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and debenzylation of)

RN 127027-65-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-bromo-7-methoxy-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 127028-09-5 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-(aminocarbonyl)-3,6,7,8-tetrahydro-4-methoxy-5-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX

NAME)

IT 127027-85-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenation of)

RN 127027-85-4 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-acetyl-3,6-dihydro-4-methoxy-5-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

IT 127027-59-2P 127027-67-2P 127027-76-3P

127027-79-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and nitration of)

RN 127027-59-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 127027-67-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-(acetyloxy)-7-methoxy-, ethyl ester (CA INDEX NAME)

RN 127027-76-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-acetyl-2,3-dihydro-7-methoxy-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

RN 127027-79-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-7-methoxy-1-[(4-methylphenyl)sulfonyl]-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

IT 127027-81-0P 127027-84-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with vinylacetate)

RN 127027-81-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-acetyl-5-(acetylhydroxyamino)-2,3-dihydro-7-methoxy-6-(phenylmethoxy)- (CA INDEX NAME)

RN 127027-84-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-(acetylhydroxyamino)-7-methoxy-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

IT 127027-77-4P 127027-80-9P 127027-95-6P

127028-07-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 127027-77-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-acetyl-2,3-dihydro-7-methoxy-5-nitro-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

RN 127027-80-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-5-nitro-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

RN 127027-95-6 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-acetyl-3,6,7,8-tetrahydro-4-methoxy-5-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 127028-07-3 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 3,6-dihydro-4-methoxy-5-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

CN 1H-Indole-2-carboxylic acid, 5-methoxy-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 67805-50-9 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-acetyl-3,6,7,8-

tetrahydro-5-hydroxy-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)

RN 70837-70-6 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-acetyl-3,6,7,8-tetrahydro-5-hydroxy-4-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 70837-76-2 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-(aminocarbonyl)-3,6,7,8-tetrahydro-5-hydroxy-4-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 127027-61-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-methoxy-7-nitro-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 127027-62-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-5-nitro-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 127027-68-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-bromo-7-methoxy-3-nitro-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & \text{O} \\ \text{Ph-CH}_2-\text{O} & \text{H} & \text{C-OEt} \\ & \text{NO}_2 & \\ & \text{Br} & \end{array}$$

RN 127027-69-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6,7-dihydro-6,7-dioxo-, ethyl ester (CA INDEX NAME)

RN 127027-70-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-4-nitro-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 127027-71-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-3-nitro-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 127027-72-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-3,4-dinitro-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

RN 127027-73-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4,7-dihydro-4,7-dioxo-, ethyl ester (CA INDEX NAME)

RN 127027-74-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-(acetyloxy)-7-methoxy-4-nitro-, ethyl ester (CA INDEX NAME)

RN 127027-78-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-acetyl-7-methoxy-5-nitro-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

RN 127027-82-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-acetyl-5-(acetylamino)-7-methoxy-6-(phenylmethoxy)-, ethenyl ester (CA INDEX NAME)

RN 127027-83-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-(acetylamino)-7-methoxy-6-(phenylmethoxy)-, ethenyl ester (CA INDEX NAME)

RN 127028-13-1 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 1-acetyl-2,3-dihydro-2-hydroxy-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 127028-14-2 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 1-acetyl-2,3-dihydro-2-hydroxy-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 127028-16-4 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 1-acetyl-, dimethyl ester (9CI) (CA INDEX NAME)

L15 ANSWER 14 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1984:33914 CAPLUS <<LOGINID::20080505>>

DN 100:33914

OREF 100:5259a,5262a

TI Photochemistry of dimethyl quinoline-3,4-dicarboxylate N-oxides

AU Irvine, Robert W.; Summers, John C.; Taylor, Walter C.

CS Dep. Org. Chem., Univ. Sydney, 2006, Australia

SO Australian Journal of Chemistry (1983), 36(7), 1419-30 CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

AB The photochem. rearrangement of di-Me 2-methyl- and 2-aryl-substituted quinoline-3,4-dicarboxylate N-oxides are examined In MeOH or MeOH-CHCl3 the major product was the 1-methyl- or 1-arylquinolin-2(1H)-one in which the substituent at C-2 has migrated to the N atom. The yield of these products was increased in a dark reaction subsequent to the irradiation In MeCN the inital major product was the corresponding 3,1-benzoxazepine; subsequent reactions yielded inter alia indole derivs. The intermediacy of fused oxaziridines or their ring opened isomeric zwitterions is discussed.

IT 54781-93-0P 88342-83-0P

RN 54781-93-0 CAPLUS

88342-83-0 CAPLUS RN

1H-Indole-2,3-dicarboxylic acid, 1-acetyl-2,3-dihydro-2-hydroxy-, dimethyl CN ester (9CI) (CA INDEX NAME)

L15 ANSWER 15 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

1982:472033 CAPLUS <<LOGINID::20080505>> AN

DN97:72033

OREF 97:12045a,12048a

Oxidation of enamine esters with lead tetraacetate. Part 2. Products from N-aryl- and N-benzylaminofumarates

ΑU Vernon, John M.; Carr, Richard M.; Sukari, Mohamed A.

CS Dep. Chem., Univ. York, York, YO1 5DD, UK

SO Journal of Chemical Research, Synopses (1982), (5), 115 CODEN: JRPSDC; ISSN: 0308-2342

DT Journal

English LA

CASREACT 97:72033 OS

GΙ

AΒ The enamines MeO2CCH:C(CO2Me)NHR (I; R = Ph, C6H3Me2-3,5, C6H4OMe-4, C6H4Cl-4, C6H4COMe-4, C6H4NO2-4, CH2Ph, Bu, cyclohexyl) and MeO2CCH:C(CO2Me)R1 (R1 = N-piperidinyl) were prepared by reaction of MeO2CC.tplbond.CCO2Me with the corresponding RNH2 and piperidine, resp., and oxidized with Pb(OAc)4. I (R = Ph, C6H3Me2-3,5) on oxidation gave dimers which eliminated amines on acid treatment to give pyrroles II (R = Ph, C6H3Me2-3,5). I (R = CH2Ph) similarly gave II (R = CH2Ph) inter alia. Treatment of I (R = C6H4Cl-4, C6H4COMe-4, C6H4NO2-4) with Pb(OAc)4 in CH2Cl2 gave the corresponding RNHCOCO2Me. This reaction involved autoxidn., as Pb(OAc)4 and air were both necessary for the formation of 4-MeCOC6H4NHCOCO2Me.

IT 969-47-1P 82633-34-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 969-47-1 CAPLUS

CN 1H-Indole-2,3,4-tricarboxylic acid, 1-methyl-, 2,3,4-trimethyl ester (CA INDEX NAME)

RN 82633-34-9 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 1-methyl-, dimethyl ester (9CI) (CA INDEX NAME)

IT 82633-35-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 82633-35-0 CAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 6-(acetyloxy)-1-methyl-, dimethyl ester (9CI) (CA INDEX NAME)

IT 82633-33-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by oxidation of indole)

RN 82633-33-8 CAPLUS

CN 3H-Indole-3,3,4-tricarboxylic acid, 5-bromo-1,2-dihydro-1-methyl-2-oxo-, trimethyl ester (9CI) (CA INDEX NAME)

L15 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1982:142623 CAPLUS <<LOGINID::20080505>>

DN 96:142623

OREF 96:23449a,23452a

TI Reactivity of 3-haloindolenines. I

AU Chun, Moon Woo; Kim, Moon Hwan

CS Coll. Pharm., Seoul Natl. Univ., Seoul, 151, S. Korea

SO Yakhak Hoechi (1981), 25(3), 83-7 CODEN: YAHOA3; ISSN: 0513-4234

DT Journal

LA Korean

AB Reaction of 3-chloroindolenine (I) with HOAc gives oxindole (II) and acetoxyindole. Similar treatment of 3-bromoindolenine (III) affords 6-bromoindole (IV). Reaction of I and III with NaOH/MeOH gives 2- and 3-methoxyindolenine and II. Thermal reaction of III in Cl2CHCHCl2 gives IV, but no reaction occurred with I. Photolysis of I gives indole and 4-, 5- and 7-chloroindole.

IT 68674-58-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with acetic acid)

RN 68674-58-8 CAPLUS

CN 3H-Indole-2-carboxylic acid, 3-chloro-3-methyl-, ethyl ester (CA INDEX NAME)

IT 14750-19-7P

RN 14750-19-7 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

L15 ANSWER 17 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1979:491436 CAPLUS <<LOGINID::20080505>>

DN 91:91436

OREF 91:14771a,14774a

TI Two novel indole rearrangements

AU Acheson, R. Morrin; Prince, Richard J.; Proctor, Garry

CS Dep. Biochem., Univ. Oxford, Oxford, UK

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1979), (3), 595-8 CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

OS CASREACT 91:91436

GI

AB Treating Et 3-methylindole-2-carboxylate with SO2Cl2 gave 35% oxoindoline I. Similar transformations accompanied by halogenation were effected by Br, or Et N,N-dichlorocarbamate in aqueous AcOH. The latter reagent converted N,N-dimethylindole-2- and -3-carboxamide into 3,5,7-trichloro-N,N-dimethyl-2-oxoindoline-3-carboxamide. Mechanisms for these amide and ester group shifts are proposed.

IT 70070-22-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and rearrangement of)

RN 70070-22-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-bromo-3-methyl-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & O \\ \parallel \\ N \\ \hline \\ Br \\ Me \end{array}$$

IT 14750-19-7P 14750-31-3P 66552-23-6P

66552-24-7P 71127-37-2P 71127-38-3P

71127-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 14750-19-7 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 14750-31-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-1-hydroxy-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 66552-23-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-bromo-3-methyl-, ethyl ester (CA INDEX NAME)

RN 66552-24-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-bromo-3-methyl-, ethyl ester (CA INDEX NAME)

RN 71127-37-2 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5-bromo-2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 71127-38-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, 4,5,6,7-tetrabromo-2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 71127-39-4 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5,7-dichloro-2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

IT 26304-51-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (rearrangement of, with sulfuryl chloride, bromine, and Et
 dichlorocarbamate)

RN 26304-51-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-methyl-, ethyl ester (CA INDEX NAME)

L15 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1978:579782 CAPLUS <<LOGINID::20080505>>

DN 89:179782

OREF 89:27915a,27918a

TI Synthesis of 3-carboethoxyoxindoles

AU Schultz, Arthur G.; Hagmann, William K.

CS Dep. Chem., Cornell Univ., Ithaca, NY, USA

SO Journal of Organic Chemistry (1978), 43(21), 4231-3

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 89:179782

GI

AB Oxindoles I (R = Me, Pr, Ph) were prepared by a simple, two-step procedure. Uranyl glass-filtered irradiation of 2-(N-methylanilino)acetoacetates in pentane solution in the presence of suspended Na2CO3 gave 3-hydroxyindolines II in quant. yield. Oxidative rearrangement of II with Pb(OAc)4 (1.1 equiv) and pyridine (1.1 equivalent) in benzene solution at room temperature gave I

(70-80% yields).

IT 67271-33-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(methylation of)

RN 67271-33-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-1-methyl-3-oxo-, ethyl ester (CA INDEX NAME)

IT 61838-88-8P 67271-26-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidative rearrangement of)

RN 61838-88-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-3-hydroxy-1,3-dimethyl-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 67271-26-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-3-hydroxy-1-methyl-3-propyl-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 39478-72-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-1-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 67271-27-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-3-hydroxy-1-methyl-3-phenyl-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 67271-28-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-1,2-dimethyl-3-oxo-, ethyl ester (CA INDEX NAME)

RN 67271-29-8 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-1,3-dimethyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 67271-30-1 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-1-methyl-2-oxo-3-propyl-, ethyl ester (CA INDEX NAME)

RN 67271-31-2 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-1-methyl-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

L15 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1978:424787 CAPLUS <<LOGINID::20080505>>

DN 89:24787

OREF 89:3861a,3864a

TI Perchloric acid, a fluorogenic spray reagent for tryptophan, tryptamine, peptides containing tryptophan and other 3-substituted indoles

AU Nakamura, Hiroshi; Pisano, John J.

CS Fac. Pharm. Sci., Univ. Tokyo, Tokyo, Japan

SO Journal of Chromatography (1978), 152(1), 167-74 CODEN: JOCRAM; ISSN: 0021-9673

DT Journal

LA English

AB When silica gel plates containing 3-substituted indoles (e.g., 3-methylindole, indole-3-acetic acid), tryptophan derivs., tryptamine, and tryptophan-containing peptides (e.g., H-Trp-Gly-OH, H-Pro-Trp-OH, H-Lys-Trp-Lys-OH) were sprayed with 70% HClO4, a strong yellow-orange

fluorescence developed. Other indole derivs, did not give this fluorescence when sprayed with 70% HClO4. 3-Substituted indoles can be detected at 40-850 pmole by this method.

IT 1477-50-5 3770-50-1 10517-21-2

16136-58-6 66866-41-9

RL: ANT (Analyte); ANST (Analytical study)

(detection of, by fluorescence on silica gel plates after spraying with perchloric acid)

RN 1477-50-5 CAPLUS

CN 1H-Indole-2-carboxylic acid (CA INDEX NAME)

RN 3770-50-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, ethyl ester (CA INDEX NAME)

RN 10517-21-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro- (CA INDEX NAME)

RN 16136-58-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-methyl- (CA INDEX NAME)

RN 66866-41-9 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2-ethoxy-5-hydroxy-, ethyl ester (CA INDEX NAME)

L15 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN ΑN

DN 79:105035

OREF 79:17027a,17030a

Synthesis and transformations of some 3-chloro- and 3-nitroindolenines ТΤ

Walser, Armin; Blount, John F.; Fryer, R. Ian ΑU

CS Chem. Res. Dep., Hoffmann-La Roche, Inc., Nutley, NJ, USA

Journal of Organic Chemistry (1973), 38(18), 3077-84 SO CODEN: JOCEAH; ISSN: 0022-3263

DTJournal

English LA

AΒ Addnl. data considered in abstracting and indexing are available from a source cited in the original document. 3-Substituted indole-2carboxylates and amides are converted to the corresponding 3-chloroindolenines by reaction with tert-butyl hypochlorite. compds. rearrange in protic solvents to oxindoles with migration of the ester or amide function into the 3 position. 3-Substituted 2-acetylindoles and indole-2-carboxylic acids are converted to the oxindoles with loss of the carbonyl function. The intermediate 2-alkoxyindoles may be isolated.

ΙT 37129-23-0

> RL: RCT (Reactant); RACT (Reactant or reagent) (nitration of)

RN 37129-23-0 CAPLUS

1H-Indole-2-carboxylic acid, 3-phenyl-, ethyl ester (CA INDEX NAME) CN

```
16381-47-8P 21139-32-2P 24106-89-6P
ΙT
     40731-20-2P 40731-21-3P 40731-22-4P
     40731-23-5P 40731-24-6P 40731-36-0P
     40735-55-5P 40735-56-6P 40735-57-7P
     40735-58-8P 40735-59-9P 40735-60-2P
     40735-61-3P 40735-62-4P 40735-63-5P
     40735-64-6P 40827-73-4P 40827-74-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     16381-47-8 CAPLUS
     1H-Indole-2-carboxylic acid, 5-chloro-3-methyl- (CA INDEX NAME)
CN
```

RN 21139-32-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 24106-89-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-3-(2-fluorophenyl)- (CA INDEX NAME)

RN 40731-20-2 CAPLUS

CN 3H-Indole-2-carboxylic acid, 3-nitro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40731-21-3 CAPLUS

CN 3H-Indole-2-carboxylic acid, 5-chloro-3-nitro-3-phenyl-, ethyl ester (CA INDEX NAME)

$$C1$$
 N
 $C-OEt$
 NO_2

RN 40731-22-4 CAPLUS

CN 3H-Indole-2-carboxylic acid, 4,7-dichloro-3-nitro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40731-23-5 CAPLUS

CN 3H-Indole-2-carboxylic acid, 6,7-dichloro-3-nitro-3-phenyl-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{O} \\ \parallel & \parallel \\ \text{C-OEt} \\ \hline & \text{NO}_2 \\ \end{array}$$

RN 40731-24-6 CAPLUS

CN 3H-Indole-2-carboxylic acid, 5,7-dimethyl-3-nitro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40731-36-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6,7-dichloro-3-phenyl- (CA INDEX NAME)

$$C1$$
 H
 CO_2H
 Ph

RN 40735-55-5 CAPLUS

CN 3H-Indole-2-carboxylic acid, 3,5-dichloro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40735-56-6 CAPLUS

CN 3H-Indole-2-carboxylic acid, 3,5-dichloro-3-(2-fluorophenyl)-, ethyl ester (CA INDEX NAME)

RN 40735-57-7 CAPLUS

CN 3H-Indole-2-carboxylic acid, 3,5-dichloro-3-methyl-, ethyl ester (CA INDEX NAME)

RN 40735-58-8 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40735-59-9 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5-chloro-2,3-dihydro-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40735-60-2 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5-chloro-3-(2-fluorophenyl)-2,3-dihydro-2-oxo-, ethyl ester (CA INDEX NAME)

RN 40735-61-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5-chloro-2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 40735-62-4 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5,7-dichloro-2,3-dihydro-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40735-63-5 CAPLUS

CN 1H-Indole-3-carboxylic acid, 4,7-dichloro-2,3-dihydro-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40735-64-6 CAPLUS

CN 1H-Indole-3-carboxylic acid, 6,7-dichloro-2,3-dihydro-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40827-73-4 CAPLUS

CN 3H-Indole-2-carboxylic acid, 5,7-dichloro-3-nitro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40827-74-5 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-5,7-dimethyl-2-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

IT 40735-51-1 40735-52-2 40735-53-3

40735-54-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with tert-butyl hypochlorite, chlorination by)

RN 40735-51-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5,7-dichloro-3-phenyl-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} C1 & O \\ H & C-OEt \\ \end{array}$$

RN 40735-52-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4,7-dichloro-3-phenyl-, ethyl ester (CA INDEX NAME)

RN 40735-53-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6,7-dichloro-3-phenyl-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} C1 & 0 \\ H & C-OEt \\ \end{array}$$

L15 ANSWER 21 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1972:539708 CAPLUS <<LOGINID::20080505>>

DN 77:139708

OREF 77:22965a,22968a

TI Migration of ethyl ester group on ethyl 3-methylindole-2-carboxylate

AU Saki, Shinichiro; Katano, Kiyoaki

CS Fac. Pharm. Sci., Chiba Univ., Chiba, Japan

SO Yakugaku Zasshi (1972), 92(9), 1129-32 CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Japanese

AB The reaction of Et 3-methylindole-2-carboxylate (I) with SO2Cl2 afforded Et 3-methyloxindole-3-carboxylate (II) and not Et 1-hydroxy-3-methylindole-2-carboxylate as previously reported by J. Elks et al. (1944). Furthermore, the reaction of I with Pb(OAc)4 gave Et 3-acetoxy-3-methyl-3-indole-2-carboxylate, which underwent rearrangement by aqueous AcOH to II.

RN 14750-19-7 CAPLUS

CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 38256-37-0 CAPLUS

CN 1H-Indole-3-carboxylic acid, 1-acetyl-2,3-dihydro-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 38256-38-1 CAPLUS

CN 3H-Indole-2-carboxylic acid, 3-(acetyloxy)-3-methyl-, ethyl ester (CA INDEX NAME)

IT 26304-51-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (rearrangement of ethyl ester group in)

RN 26304-51-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-methyl-, ethyl ester (CA INDEX NAME)

L15 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1971:488426 CAPLUS <<LOGINID::20080505>>

DN 75:88426

OREF 75:14001a,14004a

TI Chlorination of 5-methoxyindole derivatives

AU Bass, R. J.

CS Res. Div., Pfizer Ltd., Sandwich/Kent, UK

SO Tetrahedron (1971), 27(14), 3263-70 CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

OS CASREACT 75:88426

AB 5-Methoxyindole-2-carboxylic acid and its Me ester were reacted with N,N-dichlorourethane in HOAc both glacial and aqueous The probable role of water in these substitution reactions was elucidated. Novel chlorinated isatins and oxindoles were obtained and reaction mechanisms for their formation suggested.

IT 33234-31-0P 33234-32-1P 33234-35-4P

RN 33234-31-0 CAPLUS

CN 3H-Indole-2-carboxylic acid, 3,3,4-trichloro-5-methoxy-, methyl ester (CA INDEX NAME)

RN 33234-32-1 CAPLUS

CN Indole-2-carboxylic acid, 3,4-dichloro-5-methoxy- (8CI) (CA INDEX NAME)

RN 33234-35-4 CAPLUS

CN 3-Indolinecarboxylic acid, 3,4-dichloro-5-methoxy-2-oxo-, methyl ester (8CI) (CA INDEX NAME)

L15 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1970:78795 CAPLUS <<LOGINID::20080505>>

DN 72:78795

OREF 72:14341a,14344a

TI Chlorination of some indole derivatives with ethyl N,N-dichlorocarbamate

AU Muchowski, Joseph M.

CS Bristol Lab. Canada, Candiac, QC, Can.

SO Canadian Journal of Chemistry (1970), 48(3), 422-8 CODEN: CJCHAG; ISSN: 0008-4042

DT Journal

LA English

AB The sole product obtained from the reaction of indole-2-carboxylic acid and Et N,N-dichlorocarbamate was 3,3,5-trichlorooxindole. In contrast, Me indole-2-carboxylate gave a mixture of Me 3,5-dichlorooxindole-3-carboxylate and Me 3,5,7-trichlorooxindole-3-carboxylate, the same products as obtained from the chlorination of Me indole-3-carboxylate. The structures of the products were confirmed by degradation to known compounds and (or) by synthesis, and mechanisms for their formation were suggested.

IT 26450-63-5
 RL: RCT (Reactant); RACT (Reactant or reagent)

(3,3,5-trichloro-2-indolinone vs., from chlorination of indolecarboxylic acid by ethyl dichlorocarbamate)

RN 26450-63-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3,5-trichloro-2,3-dihydro-3-hydroxy-, methyl ester (CA INDEX NAME)

IT 1202-04-6 1477-50-5

RL: RCT (Reactant); RACT (Reactant or reagent) (chlorination of, by ethyl dichlorocarbamate)

RN 1202-04-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, methyl ester (CA INDEX NAME)

RN 1477-50-5 CAPLUS

CN 1H-Indole-2-carboxylic acid (CA INDEX NAME)

IT 25576-70-9

RL: RCT (Reactant); RACT (Reactant or reagent) (mixture with methyl dichloroxoindolinecarboxylate)

RN 25576-70-9 CAPLUS

CN 3-Indolinecarboxylic acid, 3,5,7-trichloro-2-oxo-, methyl ester (8CI) (CA INDEX NAME)

RN 17630-78-3 CAPLUS

CN 3-Indolinecarboxylic acid, 3,5-dichloro-2-oxo-, methyl ester (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & H & O \\ \hline & C - OMe \\ \hline & C1 & O \end{array}$$

RN 25576-71-0 CAPLUS

CN 1H-Indole-3-carboxylic acid, 5-chloro-2,3-dihydro-2-oxo-, methyl ester (CA INDEX NAME)

RN 25617-24-7 CAPLUS

CN 3-Indolinecarboxylic acid, 5,7-dichloro-2-oxo-, methyl ester (8CI) (CA INDEX NAME)

L15 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1969:449824 CAPLUS <<LOGINID::20080505>>

DN 71:49824

OREF 71:9157a,9160a

TI Additions to triple bonds. XIII. Nitrone adducts with dimethyl acetylene dicarboxylate

AU Winterfeldt, Ekkehard; Krohn, Wolfgang; Stracke, Heinz U.

CS Tech. Univ. Berlin, Berlin, Fed. Rep. Ger.

SO Chemische Berichte (1969), 102(7), 2346-61 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 71:49824

GI For diagram(s), see printed CA Issue.

AB RN(0):C(CO2Me)CH2CO2Me (R = Me or Et) (E. Winterfeldt and W. Krohn, 1969) reacted at 0° with MeO2CC.tplbond.CCO2Me to give 2-(R-substituted)-3-(carbomethoxymethyl)-3,4,5-tris(carbomethoxy)-4-isoxazoline, which kept at room temperature underwent a Cope rearrangement to give OC(CO2Me)CH(CO2Me)C(CO2Me):C(CO2Me)NHR. The reaction of PhNHOH with MeO2CC.tplbond.CCO2Me gave 2-phenyl-3-(carbomethoxymethyl)-5-(N-phenyl-N-hydroxyamino)-3,4,5-tris(carbomethoxy)isoxazolidine (I).

IT 23893-77-8P 24100-61-6P

RN 23893-77-8 CAPLUS

CN 2,3-Indolinedicarboxylic acid, 2-(carboxymethyl)-, trimethyl ester (8CI) (CA INDEX NAME)

RN 24100-61-6 CAPLUS

L15 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1969:47211 CAPLUS <<LOGINID::20080505>>

DN 70:47211

OREF 70:8847a,8850a

 ${\tt TI}$ Pseudohalogens. XII. Reaction of N,N-dichlorourethane with indole and derivatives

AU Foglia, Thomas A.; Swern, Daniel

CS Temple Univ., Philadelphia, PA, USA

SO Journal of Organic Chemistry (1968), 33(12), 4440-2 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 70:47211

AB Contrary to literature reports, the major product of reaction of C12NCO2Et (I) with indole and indole-2- or -3-carboxylic acid is 3,3,5-trichlorooxindole. Reaction of the Me esters with I yields 2-carbomethoxy-2,5,7-trichloroindoxyl and 3-carbomethoxy-3,5-dichlorooxindole, resp. Structures were assigned by phys. and chemical methods. 16 references.

IT 17630-77-2P 17630-78-3P

RN 17630-77-2 CAPLUS

CN 2-Indolinecarboxylic acid, 2,5,7-trichloro-3-oxo-, methyl ester (8CI) (CA INDEX NAME)

RN 17630-78-3 CAPLUS

CN 3-Indolinecarboxylic acid, 3,5-dichloro-2-oxo-, methyl ester (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & H & O \\ \hline & N & C \\ \hline & C & OMe \\ \hline & C1 & O \end{array}$$

L15 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1965:66385 CAPLUS <<LOGINID::20080505>>

DN 62:66385

OREF 62:11763a-q

TI Synthesis of N-containing heterocyclic compounds possessing physiological activity

AU Colwell, W. T.; Horner, J. K.; Skinner, W. A.

SO United States Department of Commerce, Office of Technical Services, PB Report (1964), AD 435,889, 33 pp.
CODEN: XCPRAL; ISSN: 0099-8567

DT Journal

LA English

AB 5-Chloroindole treated with oxalyl chloride gave 3-(5-chloroindolyl)glyoxalyl chloride (I). I with Me2NH and NH3 formed N,N-dimethyl-3-(5-chloroindole)glyoxylamide (II), m. 187.5-89°, and 3-(5-chloroindole)glyoxylamide (III), m. 292-3.5° (decomposition), resp. II and III on reduction with LiAlH4 gave 5-chloro-3-(β -dimethylaminoethyl)indole (HCl salt m. 193-3.5°) and 5-chloro-3-(β -aminoethyl)indole [HCl salt m. 277-8° (decomposition)], resp. Diazotized p-methoxyaniline on reduction gave the

```
hydrazide (IV), and the hydrazone of IV with EtMeCO was treated with H2SO4
to give 5-methoxy-2,3-dimethylindole, m. 108-12.5°. IV treated
with iso-BuMeCO (V) followed by heating with H2SO4 and EtOH gave
5-methoxy-2-methyl-3-(1-methylethyl)indole, m. 110-13°. The
hydrazone (m. 80-1^{\circ}) from V with p-nitrophenylhydrazine on heating
with concentrated HCl and C6H6 gave 2-methyl-3-(1-methylethyl)-5-nitroindole
(VI), m. 166-7.5^{\circ}. Reduction of VI gave 5-\text{amino}-2-\text{methyl}-3-(1-
methylethyl)indole, m. 124.5-5.5°. Reaction of HCONMe2 and POCl3
with 5-bromoindole and 5-chloroindole vielded 5-bromoindole- (VII, m.
200-5°) and 5-chloroindole-3-carboxaldehyde (VIII), m.
213.5-14°, resp. VII was refluxed with nitroethane in the presence
of piperidine under N in benzene to give 5-bromo-3-(2-nitropropenyl)indole
(IX), m. 220-1^{\circ}. VIII similarly gave the 5-chloro analog (X), m.
203-3.5°. IX and X on reduction with LiAlH4 yielded 5-bromo-, m.
108-9.5^{\circ} and 5-chloro-3-(2-aminopropyl)indole, m. <math>97-104^{\circ},
resp. Reaction of 5-bromoindole with HCHO and Me2NH under N gave
5-bromogramine (XI), m. 147-52^{\circ}. XI heated with 2-nitropropane and
NaOH to 110-20° under N gave 5-bromo-3-(2-methyl-2-
nitropropyl)indole (XIa), m. 109-9.5°. Gramine heated with
2-nitropropane and NaOH at 110-20^{\circ} under N gave
3-(2-methyl-2-nitropropyl) indole, m. 75-5.2^{\circ}. 3-(3-Methyl-2-
nitropropyl)indole was similarly prepared, m. 75.5-76°. Reduction of Xla
with iron filings and aqueous AcOH yielded 5-bromo- \!\alpha,\alpha\! -
dimethyltryptamine, m. 161.5-2.0°. 5-Chlorogramine, m.
.apprx.140°, prepared like XI was treated with 2-nitropropane and the
product reduced with iron filings and aqueous AcOH to yield
5-chloro-\alpha, \alpha-dimethyltryptamine, m. 156-7.5°. Aqueous K
2-piperidone-3-carboxylate was treated with diazotized 4-butylaniline to
give 2,3-piperidione 3-(4-butylphenyl)hydrazone (XII), m. 194-7°
(XII). The hydrochloride of XII was refluxed 15 min. to yield
6-butyl-1,2,3,4-tetrahydro-1-oxo-\beta-carboline (XIII), m. 150°.
XIII refluxed with aqueous KOH in ethanol gave 3-(2-aminoethyl)-5-butylindole-
2-carboxylic acid (XIV), m. 208-12°. Refluxing XIV with 2N HCl in
AcOH gave 5-butyltryptamine hydrochloride, m. 235°. Diazotized
4-benzylthioaniline was treated with K 2-piperidone-3-carboxylate and the
2,3-piperidione 3-(4-benzylthiophenyl)hydrazone, m. 203-5°, formed
was converted into the hydrochloride, which was boiled to give
6-benzylthio-1,2,3,4-tetrahydro-1-oxo-\beta-carboline (XV), m.
197-8°. XV was refluxed overnight with aqueous KOH and ethanol to give
3-(2aminoethyl)-5-benzylthioindole-2-carboxylic acid (XVI), m.
220-3°. Heating XVI with 2N HCl and AcOH gave 5-benzyl-
thiotryptamine, m. 213-14°. Reaction of EtMgBr with
4,5,6-trimethoxyisatin, m. .apprx.210° (decomposition), yielded
ethyl-4,5,6-trimethoxydioxindole, m. 132.5-3.4°.
p-Benzylthioaniline reacted with diethyl oxomalonate in HOAc under N to
give 5-benzylthio-3-carbethoxydioxindole, m. 153.5-54°, which was
dissolved in aqueous NaOH and air bubbled for 0.5\ hr. on a steam bath to give
5-benzylthioisatin, m. 181-3°. Also prepared were
5-amino-2,3,3-trimethylindolenine, m. 178°, 4,5,6-trimethoxy-3-
hydroxy-3-carbethoxyindole, m. .apprx.85°, \alpha, \alpha-dimethyltryptamine, m. 122-2.5°, 3-acetylindole, m. 189-90°, 3-indolylacetonitrile, b0.4 164°, 3-(5-bromoindolyl)acetonitrile,
m. 105-9^{\circ}, 3-(5-bromo-1-benzylindoly1) acetonitrile, m.
96-7^{\circ}, and 5-\text{chloro}-3-(2-\text{methyl}-2-\text{nitropropyl}) indole.
Structure-activity relations were discussed.
795-81-3P, 3-Indolinecarboxylic acid, 3-hydroxy-4,5,6-trimethoxy-2-
oxo-, ethyl ester 842-25-1P, Indole-2-carboxylic acid,
3-(2-aminoethyl)-5-butyl- 851-93-4P, Indole-2-carboxylic acid,
3-(2-aminoethyl)-5-(benzylthio)- 903-18-4P, 3-Indolinecarboxylic
acid, 5-(benzylthio)-3-hydroxy-2-oxo-, ethyl ester
```

RL: PREP (Preparation)

(preparation of)

RN 795-81-3 CAPLUS

CN 3-Indolinecarboxylic acid, 3-hydroxy-4,5,6-trimethoxy-2-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

RN 842-25-1 CAPLUS

CN Indole-2-carboxylic acid, 3-(2-aminoethyl)-5-butyl- (7CI, 8CI) (CA INDEX NAME)

$$^{\mathrm{H}}_{\mathrm{N}}$$
 $^{\mathrm{CO}_{2}\mathrm{H}}$ $^{\mathrm{CH}_{2}-\mathrm{CH}_{2}-\mathrm{NH}_{2}}$

RN 851-93-4 CAPLUS

CN Indole-2-carboxylic acid, 3-(2-aminoethyl)-5-(benzylthio)- (7CI, 8CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathbf{H} & \mathbf{CO_2H} \\ \hline \mathbf{Ph-CH_2-S} & \mathbf{CH_2-CH_2-NH_2} \end{array}$$

RN 903-18-4 CAPLUS

CN 3-Indolinecarboxylic acid, 5-(benzylthio)-3-hydroxy-2-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

L15 ANSWER 27 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1964:469028 CAPLUS <<LOGINID::20080505>>

DN 61:69028 OREF 61:11957g-h

- TI Addition reactions of heterocyclic compounds. XX. The bromination and rearrangement of trimethyl 1-methylindole- 2,3,4-tricarboxylate
- AU Acheson, R. M.; Snaith, R. W.; Vernon, J. M.
- CS Univ. Oxford, UK
- SO Journal of the Chemical Society (1964), (Sept.), 3229-33 CODEN: JCSOA9; ISSN: 0368-1769
- DT Journal
- LA Unavailable
- GI For diagram(s), see printed CA Issue.
- AB cf. CA 61, 11880α . Trimethyl 1-methyl-indole-2,3,4-tricarboxylate with Br in aqueous AcOH gave trimethyl 5-bromo-1-methyloxindole-3,3,4-tricarboxylate (I), the structure of which was established from spectral comparisons and by step-wise degradation to 1-methyloxindole. The mechanism of the 1,2-ester shift is discussed.
- IT 93432-32-7
 - (Derived from data in the 7th Collective Formula Index (1962-1966))
- RN 93432-32-7 CAPLUS
- CN Indole-2,3,4-tricarboxylic acid, 6-bromo-1-methyl-, trimethyl ester (7CI) (CA INDEX NAME)

- IT 969-47-1, Indole-2,3,4-tricarboxylic acid, 1-methyl-, trimethyl ester
 - (bromination and rearrangement of)
- RN 969-47-1 CAPLUS
- CN 1H-Indole-2,3,4-tricarboxylic acid, 1-methyl-, 2,3,4-trimethyl ester (CA INDEX NAME)

IT 82633-33-8P, 3,3,4-Indolinetricarboxylic acid, 5-bromo-1-methyl-2-oxo-, trimethyl ester 92022-63-4P, Indole-2,4-dicarboxylic acid, 3,6-dibromo-1-methyl-, dimethyl ester 92022-64-5P, 3,4-Indolinedicarboxylic acid, 3,5-dibromo-1-methyl-2-oxo-, dimethyl ester 92060-17-8P, 3,4-Indolinedicarboxylic acid, 3,5,6-tribromo-1-methyl-2-oxo-, dimethyl ester 92851-95-1P,

3,3,4-Indolinetricarboxylic acid, 1-methyl-2-oxo-, trimethyl ester 97026-40-9P, 3,4-Indolinedicarboxylic acid, 5-bromo-1-methyl-2-oxo-, dimethyl ester RL: PREP (Preparation) (preparation of) RN 82633-33-8 CAPLUS CN 3H-Indole-3,3,4-tricarboxylic acid, 5-bromo-1,2-dihydro-1-methyl-2-oxo-, trimethyl ester (9CI) (CA INDEX NAME)

RN 92022-63-4 CAPLUS
CN Indole-2,4-dicarboxylic acid, 3,6-dibromo-1-methyl-, dimethyl ester (7CI)
(CA INDEX NAME)

RN 92022-64-5 CAPLUS CN 3,4-Indolinedicarboxylic acid, 3,5-dibromo-1-methyl-2-oxo-, dimethyl ester (7CI) (CA INDEX NAME)

RN 92060-17-8 CAPLUS CN 3,4-Indolinedicarboxylic acid, 3,5,6-tribromo-1-methyl-2-oxo-, dimethyl

RN 92851-95-1 CAPLUS

CN 3,3,4-Indolinetricarboxylic acid, 1-methyl-2-oxo-, trimethyl ester (7CI) (CA INDEX NAME)

RN 97026-40-9 CAPLUS

CN 3,4-Indolinedicarboxylic acid, 5-bromo-1-methyl-2-oxo-, dimethyl ester (7CI) (CA INDEX NAME)

L15 ANSWER 28 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1964:23245 CAPLUS <<LOGINID::20080505>>

DN 60:23245

OREF 60:4088h,4089a-c

TI Reaction of indole derivatives with thionyl and sulfuryl chlorides

AU Szmuszkovicz, Jacob

CS Upjohn Co., Kalamazoo, MI

SO Journal of Organic Chemistry (1964), 29(1), 178-84

```
CODEN: JOCEAH; ISSN: 0022-3263
     Journal
DT
LA
    Unavailable
OS
    CASREACT 60:23245
GΙ
     For diagram(s), see printed CA Issue.
     Reaction of 1-methylindole-2-carboxylic acid, the corresponding methyl
AΒ
     ester (I), and of Et indole-2-carboxylate with thionyl chloride afforded
     sulfinyl chlorides (II, III, and IV, resp.). Thionyl chloride and
     N, 1-dimethylindole-2-carboxamide led to sulfide (V, R = CONHMe) and imide
     sulfoxide (VI). III was converted to several sulfinamides (VII) on
     treatment with amines. VII were oxidized with permanganate to
     sulfonamides (VIII). Treatment of III with hydrazine in the cold gave
     disulfide (IX, R = CO2Me) (X), which was transformed to IX (R = CONHNH2)
     on heating with hydrazine. Monosulfide (V, R = CO2Me), disulfide X, and
     trisulfide XI were obtained from the reaction of I with sulfur
     monochloride. Reaction of 1-methylindole-2-carboxylic acid hydrazide with
     sulfuryl chloride led to the dichloro compound (XII), and I with sulfuryl
     chloride afforded the tetrachloro compound (XIII) and the hexachloro compound
     (XIV).
     3678-04-4P, Indole-2-carboxylic acid, 3-
ΤT
     [(butylcarbamoyl)sulfamoyl]-1-methyl- 3678-05-5P,
     Indole-2-carboxylic acid, 1-methyl-3-sulfamoyl-, methyl ester
     3678-09-9P, Indole-2-carboxylic acid, 3,3'-dithiobis[1-methyl-,
     dimethyl ester 3678-10-2P, Indole-2-carboxylic acid,
     3-(chlorosulfinyl)-1-methyl-, methyl ester 3835-62-9P,
     Indole-2-carboxylic acid, 3-(aminosulfinyl)-1-methyl-, methyl ester
     3954-44-7P, Indole-2-carboxylic acid, 3-
     [(butylcarbamoyl)sulfamoyl]-1-methyl-, methyl ester 7272-69-7P,
     Indole-2-carboxylic acid, 1-methyl-3-(piperidinosulfinyl)-, methyl ester
     7272-70-0P, Indole-2-carboxylic acid, 3-(aminosulfinyl)-, ethyl
     ester 7273-26-9P, Indole-2-carboxylic acid, 1-methyl-3-
     [(methylamino)sulfinyl]-, methyl ester 7273-27-0P,
     Indole-2-carboxylic acid, 3-[(dimethylamino)sulfinyl]-1-methyl-, methyl
     ester 82633-33-8P, 3,3,4-Indolinetricarboxylic acid,
     5-bromo-1-methyl-2-oxo-, trimethyl ester 88613-08-5P,
     Indole-2-carboxylic acid, 1-methyl-3-sulfino-, dimethyl ester
     91088-34-5P, Indole-2-carboxylic acid, 3-sulfamoyl-, ethyl ester
     91349-20-1P, Indole-2-carboxylic acid, 3-(chlorosulfinyl)-, ethyl
     ester 91567-95-2P, Indole-2-carboxylic acid,
     1-methyl-3-(methylsulfamoyl)-, methyl ester 92109-30-3P,
     Indole-2-carboxylic acid, 3-(dimethylsulfamoyl)-1-methyl-, methyl ester
     93538-46-6P, Indole-2-carboxylic acid, 1-methyl-3-
     (piperidinosulfonyl)-, methyl ester 94691-31-3P,
     Indole-2-carboxylic acid, tetrachloro-1-methyl-, methyl ester
     94691-32-4P, 2-Indolinecarboxylic acid, hexachloro-1-methyl-,
     methyl ester 95006-41-0P, Indole-2-carboxylic acid,
     3,3'-trithiobis[1-methyl-, dimethyl ester 95006-48-7P,
     Indole-2-carboxylic acid, 3,3'-sulfinylbis[1-methyl-, dimethyl ester
     95006-49-8P, Indole-2-carboxylic acid, 3,3'-sulfinyldi-, diethyl
     ester 95706-97-1P, 2-Indolinecarboxylic acid,
     trichloro-2-methoxy-1-methyl-3-oxo-, methyl ester 96171-80-1P,
     Indole-2-carboxylic acid, 3,3'-thiobis[1-methyl-, dimethyl ester
     97062-57-2P, Indole-2-carboxylic acid, 1-methyl-3-sulfeno-,
     2-methyl ester
     RL: PREP (Preparation)
        (preparation of)
RN
     3678-04-4 CAPLUS
CN
     Indole-2-carboxylic acid, 3-[(butylcarbamoyl)sulfamoyl]-1-methyl- (7CI,
     8CI) (CA INDEX NAME)
```

RN 3678-05-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-(aminosulfonyl)-1-methyl-, methyl ester (CA INDEX NAME)

RN 3678-09-9 CAPLUS

CN Indole-2-carboxylic acid, 3,3'-dithiobis[1-methyl-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)

RN 3678-10-2 CAPLUS

CN Indole-2-carboxylic acid, 3-(chlorosulfinyl)-1-methyl-, methyl ester (7CI, 8CI) (CA INDEX NAME)

RN 3835-62-9 CAPLUS

CN Indole-2-carboxylic acid, 3-(aminosulfinyl)-1-methyl-, methyl ester (7CI, 8CI) (CA INDEX NAME)

RN 3954-44-7 CAPLUS

CN Indole-2-carboxylic acid, 3-[(butylcarbamoyl)sulfamoyl]-1-methyl-, methyl ester (7CI, 8CI) (CA INDEX NAME)

RN 7272-69-7 CAPLUS

CN Indole-2-carboxylic acid, 1-methyl-3-(piperidinosulfinyl)-, methyl ester (7CI, 8CI) (CA INDEX NAME)

RN 7272-70-0 CAPLUS

CN Indole-2-carboxylic acid, 3-(aminosulfinyl)-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

RN 7273-26-9 CAPLUS

CN Indole-2-carboxylic acid, 1-methyl-3-[(methylamino)sulfinyl]-, methyl ester (7CI, 8CI) (CA INDEX NAME)

RN 7273-27-0 CAPLUS

CN Indole-2-carboxylic acid, 3-[(dimethylamino)sulfinyl]-1-methyl-, methyl ester (7CI, 8CI) (CA INDEX NAME)

RN 82633-33-8 CAPLUS

CN 3H-Indole-3,3,4-tricarboxylic acid, 5-bromo-1,2-dihydro-1-methyl-2-oxo-, trimethyl ester (9CI) (CA INDEX NAME)

RN 88613-08-5 CAPLUS

CN Indole-2-carboxylic acid, 1-methyl-3-sulfino-, dimethyl ester (7CI) (CA INDEX NAME)

RN 91088-34-5 CAPLUS

CN Indole-2-carboxylic acid, 3-sulfamoyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 91349-20-1 CAPLUS

CN Indole-2-carboxylic acid, 3-(chlorosulfinyl)-, ethyl ester (7CI) (CA INDEX NAME)

RN 91567-95-2 CAPLUS

CN Indole-2-carboxylic acid, 1-methyl-3-(methylsulfamoyl)-, methyl ester (7CI) (CA INDEX NAME)

RN 92109-30-3 CAPLUS

RN 93538-46-6 CAPLUS

CN Indole-2-carboxylic acid, 1-methyl-3-(piperidinosulfonyl)-, methyl ester (7CI) (CA INDEX NAME)

RN 94691-31-3 CAPLUS

CN Indole-2-carboxylic acid, tetrachloro-1-methyl-, methyl ester (7CI) (CA INDEX NAME)

$$4 (D1-C1)$$

6 (D1
$$-$$
C1)

RN 95006-49-8 CAPLUS

CN Indole-2-carboxylic acid, 3,3'-sulfinyldi-, diethyl ester (7CI) (CA INDEX NAME)

RN 95706-97-1 CAPLUS

CN 2-Indolinecarboxylic acid, trichloro-2-methoxy-1-methyl-3-oxo-, methyl ester (7CI) (CA INDEX NAME)

3 (D1-C1)

RN 96171-80-1 CAPLUS

CN Indole-2-carboxylic acid, 3,3'-thiobis[1-methyl-, dimethyl ester (7CI) (CA INDEX NAME)

RN 97062-57-2 CAPLUS

CN Indole-2-carboxylic acid, 1-methyl-3-sulfeno-, 2-methyl ester (7CI) (CA INDEX NAME)

L15 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1958:104210 CAPLUS <<LOGINID::20080505>>

DN 52:104210

OREF 52:18371b-i,18372a-g

TI Mescaline analogs. VIII. Substituted 5-methoxy- and 5,6,7-trimethoxyindoles

AU Benington, F.; Morin, R. D.; Clark, Leland C., Jr.

CS Battelle Mem. Inst., Columbus, O.

SO Journal of Organic Chemistry (1958), 23, 19-23 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

OS CASREACT 52:104210

aB cf. C.A. 52, 1938c, 2834g. Cyclization of appropriately substituted open chain amines gave various 5-methoxy- and 5,6,7-trimethoxyindole derivs. for use in the preparation of certain key compds. needed for examination of the indole hypothesis of psychotomimetic drug activity. Various routes were investigated for the preparation of the chosen intermediate, 2,3,4-(MeO)3C6H2NH2 (I). Oxidation of 2,3,4-(MeO)3C6H2Ac with NaOCl resulted in considerable nuclear halogenation and accordingly, preparation of I from 2,3,4-(MeO)3C6H2CONH2 by the Hoffmann reaction was abandoned. Nitration of pyrogallol carbonate according to Einhorn [Ber. 37, 100(1904)], saponification to 4-nitropyrogallol and treatment of the product with

alkaline Me2SO4 or CH2N2 in Et2O failed to give a completely methylated product. Both routes evidently give compds. soluble in dilute NaOH and containing

```
free phenolic OH groups. Ac20 (155 ml.) and 130 g. 2,6-(MeO)2C6H3OH
     refluxed 3.5 hrs. and the mixture evaporated in vacuo yielded 99%
     2,6-(MeO)\,2C6H3OAc, b1.5\,118-19^{\circ}. Concentrated HNO3 (195 ml.) and 21.7
     ml. white fuming HNO3 treated dropwise in 40 min. with 65 g. acetate at
     13-16° and the mixture stirred 10 min., poured into 1080 ml. ice H20
     containing urea, filtered, and the dried product (54.2 \text{ g., m. } 90-2^{\circ})
     recrystd. (dilute alc.) gave pure 5,2,6-02N(MeO)2C6H2OAc, m. 94-5°,
     refluxed (47 q.) in 2N NaOH 30 min. and the cooled solution acidified with
     225 ml. 10% HCl to give 39.3 q. 5,2,6-02N(MeO)2C6H3OH.2H2O, m.
     67-9°, methylated in 50 ml. alc. by adding 65 ml. Me2SO4 and
     gradually treating the cooled solution with 35 g. NaOH in 40 ml. H2O, diluting
     with 500 ml. cold H2O, and cooling to 0^{\circ} to give 38 g.
     2,3,4-(MeO)\ 3C6H2NO2\ (II),\ m.\ 44-5^{\circ}.\ SnC112.2H2O\ (160\ g.)\ and\ 160
     ml. concentrated HCl stirred at 0^{\circ} with addition of 37.9 g. II with rise of
     temperature to 97^{\circ} and the solution cooled (ice-bath) to room temperature, the
     solution treated with 285 g. NaOH and diluted with a large volume of H2O, the
     mixture exhaustively extracted with Et20 and the dried (MgSO4) extract
filtered,
     evaporated, and the residue distilled in vacuo gave 26.9 g. I, b0.8
     111-14°. Various trimethoxyindoles were prepared from I. I (34.7
     g.) and 22.7 g. CHBr(CO2Et)2 refluxed 11 hrs. in 100 ml. dry pure C6H6 and
     the mixture kept overnight at room temperature, filtered from I HBr salt (16.5
     and the concentrated filtrate cooled and filtered from 3.6 q. I HBr salt, the
     filtrate evaporated in vacuo, and the crude phenylaminomalonic ester distilled
     a high vacuum gave 700 mg. 2-carbethoxy-5,6,7-trimethoxyindoxyl (III), m.
     118-19° (C6H6-ligroine). OC(CO2Et)2 condensed smoothly with 3,4,5-(MeO)3C6H2NH2 (C.A. 50, 9381a). I (1.8 g.) in 10 ml. AcOH and 1.9
     g. OC(CO2Et)2 heated 10 min. on a steam bath and the solution kept 2 hrs. at
     room temperature, diluted with 125 ml. H2O and adjusted to pH 8 with solid
     (NH4)2CO3, the oily product taken up in Et2O, and the dried (MgSO4) extract
     evaporated yielded 700 mg. pure 3-carbethoxy-3-hydroxy-5,6,7-
     trimethoxyoxindole, C14H17NO7, m. 142-3° (Et20-petr. ether). I HBr
     salt (13.2 g.) in 30 ml. H2O treated with 25 ml. 25% NaOH and extracted with
     Et20, the dried (CaCl2) extract evaporated (N atmospheric) and the residue
refluxed 12
     min. with 5.3 q. BzH in 6 ml. alc., the cooled mixture filtered, and the
     solid recrystd. (alc.-H2O) gave 11.8 g. 2,3,4-(MeO)3C6H2N:CHPh (IV), m.
     104-5°. IV (11 g.) in 66 ml. dioxane (prereduced over Raney Ni)
     hydrogenated 13-15 min. at 30 lb./sq. in. in a Parr hydrogenation apparatus and
     the filtered solution evaporated in vacuo, the residue diluted with 125 ml.
H20.
     and extracted with Et2O gave 9.5 g. 2,3,4-(MeO)3C6H2NHCH2Ph (V), m.
     63-4^{\circ} (95% alc.). V (2.0 g.) and 1.22 g. OC(CO2Et)2.2H2O heated 10
     min. on a steam bath in 8 ml. AcOH and kept 20 min. at room temperature,
diluted
     with H2O and made alkaline, extracted with Et2O, and the product crystallized
(alc.)
     (Norit) yielded 54% 1-benzyl-3-carbethoxy-5,6,7-trimethoxydioxindole,
     C21H23NO7, m. 185-6°. V with BrCH2CH2Cl did not give the expected
     2,3-dehydroindole which, on hydrogenolysis should yield
     5,6,7-trimethoxy-2,3-dihydroindole, a possible oxidative cyclization
     product of mescaline (C.A. 52, 2834g). V (3.0 g.) in 15 ml. BrCH2CH2Cl
     refluxed 15 hrs. and the mixture treated with 10% HCl, the mixture steam
     distilled and the clear distillate made strongly alkaline with 20% NaOH,
extracted 3
     times with Et20, and the product (250 mg., m. 172-3^{\circ}) sublimed in a
     high vacuum gave N,N'-bis(2,3,4-trimethoxyphenyl)piperazine, m.
     176-7°. V was unchanged through reaction with glyoxal Na bisulfite
```

(cf. Burton, C.A. 26, 2456) and with chloral hydrate and HONH2 gave an

g.)

in

intractable tar. Both p-MeOC6H4NHCH2Ph (VI) and p-MeOC6H4NHMe (VII) were examined in connection with their tendencies to form isatins which might be converted to indole derivs. BzH (21.2 g.) added to 24.6 g. p-MeOC6H4NH2 in 20 ml. alc. and warmed 10 min. on a steam bath, the cooled mixture filtered, and the Schiff base recrystd. (alc.) gave 34.5 g. pure p-Me-OC6H4N:CHPh, m. 73-4°, hydrogenated (33.2 g.) in dioxane with Raney Ni 13-15 min. at 30 lb./sq. in. to give 31.3 g. VI. VI (3.0 g.) in 8.4 ml. H2O containing 1.5 ml. concentrated HCl poured into 33 ml. H2O containing 3.0 g.

CCl3CHO.H2O and 31 g. Na2SO4.10H2O and the mixture heated 20 min. on a steam bath with 3.1 g. HONH2.HCl in 14 ml. H2O, the cooled mixture decanted and the oily layer taken up in EtOAc, the solution decolorized (Norit) and the filtered solution concentrated, the cooled concentrate filtered, and the precipitate

recrystd. (EtOAc) gave 200 mg. N,N'-bis(4-methoxyphenyl)-N,N'-bis-(benzyloxamide), C30H28N2O4, m. 179-80°. N-Formylation of p-MeOC6H4NH2 with 90% HCO2H yielded 91% p-Me-OC6H4NHCHO (VIII), b0.5 156-9°, m. 84-5°. VIII (37.8 g.) in 150 ml. hot dry C6H6 gradually added to 14.2 g. LiAlH4 in 250 ml. dry Et2O and the mixture refluxed 1 hr., hydrolyzed by cautious addition of H2O and the filtered organic layer dried (anhydrous MgSO4), the extract evaporated in vacuo, and distilled gave 27.8

 $q. VII, b0.2 80-4^{\circ}, m. 35^{\circ}. CC13CHO.H2O (18 q.) and 260 q.$ Na2SO4.10H2O in 240 ml. H2O and 13.7 g. VII in 60 ml. H2O containing 8.6 ml. concentrated HCl heated 15-20 min. on a steam bath with 22 g. HONH2.HCl in 100 ml. H2O and the cooled solution filtered, the dried product (11.5 g.) taken up in AcOEt and decolorized (Norit), diluted with petr. ether, and filtered gave p-MeOC6H4NMeCOCH:NOH (IX), C10H12N2O3.H2O, m. 116-17°. Concentrated $\rm H2SO4$ (40 ml.) at 50° on a steam bath, treated with 9.6 g. IX at a rate maintaining the temperature at $60-70^{\circ}$ and the blue-violet solution kept 10 min. at 80° , cooled to room temperature and poured onto 450 cracked ice, filtered and the product washed acid-free with H2O, dried, and the product (7.2 g., m. 175-6°) recrystd. (MeOH-H2O) gave 5-methoxy-1-methylisatin, m. 176°; this stirred in 30 ml. boiling H2O with 7.0 g. NaHSO3, and the clear solution refrigerated overnight, filtered, and the dried product (4.9 g., m. 158-60°) recrystd. (boiling H2O) yielded pure 5-methoxy-1-methyldioxindole (X), m. 165°. LiAlH4 (1.9 g.) stirred vigorously in 100 ml. dry Et20 with addition of 3.3 q. X in 120 ml. dry C6H6 and the mixture refluxed 3.75 hrs., cooled to 0° and hydrolyzed with a small amount of H2O, the filtered organic layer dried (MgSO4) and evaporated in vacuo, refrigerated, and the product (2.2 g., m. 75-80°) recrystd. (Et20-petr. ether) yielded 900 mg. 5-methoxy-1-methylindole, m. 104-5°; picrate, m. 98-100° (cf. Bell and Lindwall, C.A. 44, 604a).

IT 100719-35-5P, 2-Indolinecarboxylic acid, 5,6,7-trimethoxy-3-oxo-, ethyl ester 100719-43-5P, 3-Indolinecarboxylic acid, 3-hydroxy-5,6,7-trimethoxy-2-oxo-, ethyl ester 102449-85-4P, 3-Indolinecarboxylic acid, 1-benzyl-3-hydroxy-5,6,7-trimethoxy-2-oxo-, ethyl ester

RL: PREP (Preparation) (preparation of)

RN 100719-35-5 CAPLUS

CN 2-Indolinecarboxylic acid, 5,6,7-trimethoxy-3-oxo-, ethyl ester (6CI) (CA INDEX NAME)

RN 100719-43-5 CAPLUS

CN 3-Indolinecarboxylic acid, 3-hydroxy-5,6,7-trimethoxy-2-oxo-, ethyl ester (6CI) (CA INDEX NAME)

RN 102449-85-4 CAPLUS

CN 3-Indolinecarboxylic acid, 1-benzyl-3-hydroxy-5,6,7-trimethoxy-2-oxo-, ethyl ester (6CI) (CA INDEX NAME)

L15 ANSWER 30 OF 30 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1956:48695 CAPLUS <<LOGINID::20080505>>

DN 50:48695

OREF 50:9381a-d

TI Mescaline analogs. IV. Substituted 4,5,6-trimethoxyindoles

AU Benington, F.; Morin, R. D.; Clark, Leland C., Jr.

CS Battelle Memorial Inst., Columbus, O.

SO Journal of Organic Chemistry (1955), 20, 1454-7 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

cf. C.A. 50, 8497i. Trimethylgalloyl chloride and NH3 give 100% 3,4,5-(MeO)3C6H2CONH2, which (80 g.), added to a NaOCl solution (prepared by passing 28.3 g. Cl into 590 cc. H2O containing 95 g. NaOH and 360 g. ice), the temperature allowed to rise to 65-70° within 1 hr., 130 g. NaOH in 130 cc. H2O added, and the mixture kept another hr. at 700 gives 66% 3,4,5-(MeO)3C6H2NH2 (I), m. 116-18°. Refluxing 4 hrs. 36.6 g. I and 23.9 g. CHBr(CO2Et)2 in 125 cc. C6H6 gives 50% 3,4,5-(MeO)3C6H2NHCH(CO2Et)2 (II), m. 103-4°. Adding with stirring 9.9

g. II to 46 cc. Nujol preheated to $245-50^{\circ}$, keeping the mixture 0.75hr. at $240-50^{\circ}$, taking up the precipitate in Et20, and recrystg. the residue of the Et2O solution gives 14% Et 4,5,6-trimethoxyindoxyl-2carboxylate, yellow prisms, m. 168-9°, which, methylated with Me2SO4 and 2N KOH, yields 41% 3,4,5,6-tetramethoxy-2-carbethoxyindole, greenish white needles, m. 135-6°. Treating 1.8 g. I in 10 cc. AcOH with 1.9 g. CO(CO2Et)2.2H2O 10 min. on a steam bath and 2 hrs. at 20° gives 86.8% 4,5,6-trimethoxy-3-hydroxy-3-carbethoxyoxindole (III), prisms, m. 189-90°. Passing air into 450 mg. III in 5 cc. 5% NaOH 10 min. and adjusting the pH of the mixture to 4 with 95% HCO2H gives 100 mg. 4,5,6-trimethoxyisatin, orange platelets, m. 194-5° (decomposition). Refluxing 40 hrs. 1.4 g. I and 7.3 cc. Cl(CH2)2Br, adding dilute HCl, and steam-distilling the mixture, then adding a large excess of 20% NaOH and extracting with Et20-CHCl3 gives 400 mg. 1,4-bis(3,4,5trimethoxyphenyl)piperazine, prisms, m. 201-2°, which is not benzoylated or acetylated by the usual methods. Refluxing 7.2 g. I, 4.8 g. CH2ClCOCl, and 60 cc. Me2CO 72 hrs., pouring the mixture into dilute HCl, and extracting with Et20 gives 68% 3,4,5-(MeO)3C6H2NHCOCH2Cl, m. $119-20^{\circ}$, which fails to undergo a catalytic cyclization to the 2,3-dihydroindole.

TT 795-81-3P, 3-Indolinecarboxylic acid, 3-hydroxy-4,5,6-trimethoxy-2-oxo-, ethyl ester 855604-65-8P, 2-Indolinecarboxylic acid, 4,5,6-trimethoxy-3-oxo-, ethyl ester 858233-74-6P, 2-Indolecarboxylic acid, 3,4,5,6-tetramethoxy-, ethyl ester RL: PREP (Preparation) (preparation of)

795-81-3 CAPLUS

CN 3-Indolinecarboxylic acid, 3-hydroxy-4,5,6-trimethoxy-2-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

RN 855604-65-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 2,3-dihydro-4,5,6-trimethoxy-3-oxo-, ethyl ester (CA INDEX NAME)

RN 858233-74-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3,4,5,6-tetramethoxy-, ethyl ester (CA INDEX NAME)